CMOS Compatible Thin-Film ALD Tungsten Nanoelectromechanical Devices

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CMOS Compatible Thin-Film ALD Tungsten Nanoelectromechanical Devices

by

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B.S. Mechanical Engineering, University of Colorado, 2006
M.S. Mechanical Engineering, University of Colorado, 2008

A thesis submitted to the
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Department of Mechanical Engineering
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This thesis entitled:
CMOS Compatible Thin-Film ALD Tungsten Nanoelectromechanical Devices
written by
Bradley Darren Davidson
has been approved for the Department of Mechanical Engineering

Prof. Victor M. Bright

Prof. Scott Bunch

Prof. Y.C. Lee

Prof. Bart Van Zeghbroeck

Prof. Li Shang

Date ________________

The final copy of this thesis has been examined by the signatories, and we find that both the content and the form meet acceptable presentation standards of scholarly work in the above mentioned discipline.
This research focuses on the development of a novel, low-temperature, CMOS compatible, atomic-layer-deposition (ALD) enabled NEMS fabrication process for the development of ALD Tungsten (WALD) NEMS devices. The devices are intended for use in CMOS/NEMS hybrid systems, and NEMS based micro-processors/controllers capable of reliable operation in harsh environments not accessible to standard CMOS technologies.

The majority of NEMS switches/devices to date have been based on carbon-nano-tube (CNT) designs. The devices consume little power during actuation, and as expected, have demonstrated actuation voltages much smaller than MEMS switches. Unfortunately, NEMS CNT switches are not typically CMOS integrable due to the high temperatures required for their growth, and their fabrication typically results in extremely low and unpredictable yields. Thin-film NEMS devices offer great advantages over reported CNT devices for several reasons, including: higher fabrication yields, low-temperature (CMOS compatible) deposition techniques like ALD, and increased control over design parameters/device performance metrics, i.e., device geometry. Furthermore, top-down, thin-film, nano-fabrication techniques are better capable of producing complicated device geometries than CNT based processes, enabling the design and development of multi-terminal switches well-suited for low-power hybrid NEMS/CMOS systems as well as electromechanical transistors and logic devices for use in temperature/radiation hard computing architectures.

In this work several novel, low-temperature, CMOS compatible fabrication technologies, employing WALD as a structural layer for MEMS or NEMS devices, were developed. The technologies developed are top-down nano-scale fabrication processes based on traditional micro-machining techniques commonly used in the fabrication of MEMS devices.
Using these processes a variety of novel WALD NEMS devices have been successfully fabricated and characterized. Using two different WALD fabrication technologies two generations of 2-terminal WALD NEMS switches have been developed. These devices have functional gap heights of 30-50 nm, and actuation voltages typically ranging from 3-5 Volts. Via the extension of a two terminal WALD technology novel 3-terminal WALD NEMS devices were developed. These devices have actuation voltages ranging from 1.5-3 Volts, reliabilities in excess of 2 million cycles, and have been designed to be the fundamental building blocks for WALD NEMS complementary inverters.

Through the development of these devices several advancements in the modeling and design of thin-film NEMS devices were achieved. A new model was developed to better characterize pre-actuation currents commonly measured for NEMS switches with nano-scale gate-to-source gap heights. The developed model is an extension of the standard field-emission model and considers the electromechanical response, and electric field effects specific to thin-film NEMS switches. Finally, a multi-physics FEM/FD based model was developed to simulate the dynamic behavior of 2 or 3-terminal electrostatically actuated devices whose electrostatic domains have an aspect ratio on the order of $10^{-3}$. The model uses a faux-Lagrangian finite difference method to solve Laplace's equation in a quasi-statically deforming domain. This model allows for the numerical characterization and design of thin-film NEMS devices not feasible using typical non-specialized BEM/FEM based software. Using this model several novel and feasible designs for fixed-fixed 3-terminal WALD NEMS switches capable for the construction of complementary inverters were discovered.
Dedication

I would like to dedicate this work to anyone that has been told that they cannot do something, those who laud respect education, knowledge, logic, honesty and perseverance; and anyone who has ever devoted themselves entirely to pursuit of their own dreams, passions, and happiness – whatever they may be.

*In reality we have nothing to lose but everything to gain.*
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## Contents

### Chapter

1. **Introduction**
   - 1.1 Motivation ...................................................... 1
   - 1.2 Scope and Application ........................................ 2
   - 1.3 Achievements ................................................... 4
   - 1.4 Organization of Dissertation ................................. 6

2. **Literature Review and the State-of-the-art**
   - 2.1 ALD .............................................................. 9
     - 2.1.1 WALD ...................................................... 12
     - 2.1.2 ALD use in MEMS and NEMS to Date ................. 13
     - 2.1.3 W use in MEMS/NEMS .................................. 15
   - 2.2 Electrostatic Micro/Nano Mechanical Switches and Logic Devices .......... 19
     - 2.2.1 MEMS Switches ........................................... 19
     - 2.2.2 MEMS State-Of-The-Art Electrostatically Actuated Switches ........ 22
     - 2.2.3 NEMS ....................................................... 23
     - 2.2.4 Carbon Nano-tube (CNT) Based NEMS Switches ........... 24
     - 2.2.5 Thin-film (TF) Based NEMS Switches .................... 28
     - 2.2.6 State-of-the-Art Graphene Based NEMS Switches ........ 31
     - 2.2.7 MEMS and NEMS Logic .................................. 33
     - 2.2.8 State-of-the-Art MEMS and NEMS Logic ................ 35
Relevant Analytic and Computational Modeling for the Design of Thin-film NEMS Switches having Symmetric, Non-Rectangular Profiles

3.1 Overview

3.2 Effective Stiffness of Two or Three Terminal MEMS/NEMS Switches having Symmetric Non-Rectangular Profiles

3.2.1 Rectangular Profiles

3.2.2 Section 1: $0 \leq x < a$

3.2.3 Section 2: $a < x \leq L$

3.2.4 Fixed-fixed Beam Subjected to a Fully-Distributed Load

3.2.5 Non-rectangular Profiles

3.2.6 Partially Distributed Loads

3.3 Pull-in of 2 or 3 Terminal Bow/Poly-tie MEMS/NEMS Switches

3.3.1 Analytic Case Studies: Displacement Vs. Applied Voltage for Rectangular, Bow-tie, and 2nd Order Poly-tie WALD NEMS 2 and 3-terminal Switches

3.4 Non-linear Dynamics of Electromechanical System Including van der Waals Force

3.4.1 Equations of Motion

3.4.2 Analysis of the Static System

3.4.3 Analysis of the Non-Linear System Dynamics

3.4.4 van der Waals Detachment Length

3.5 Tunneling Current

3.5.1 Electron Tunneling

3.5.2 Field Emission Current Density

3.5.3 Approximation of Electric Field Strength at Thin-Film Corners

3.5.4 Extended Field Emission/Tunneling Current Model For MEMS/NEMS Electrostatically Actuated Devices
3.5.5 Theoretical Case studies ............................................ 103

4 Computational Modeling: 2-D Multi-Physics FLFD/FEM Model for Electromechanically Actuated NEMS Switches With Aspect Ratios $< 10^{-2}$ .......................................................... 108

4.1 Overview ................................................................. 108

4.2 Computational Modeling in MEMS ...................................... 109

4.2.1 The Mixed FEM/BEM Method ........................................ 110

4.3 Euler-Lagrange FE Formulation of the Mechanical Domain .......... 111

4.4 Formulation of the Faux-Lagrangian Finite Difference Solver for application to Electrostatics/Potential Problems .......................................................... 116

4.4.1 Governing Equations .................................................. 116

4.4.2 The Faux-Lagrangian Finite Difference Scheme ....................... 118

4.4.3 Average Radial Distances for Special Boundaries ..................... 123

4.4.4 Application of Boundary Conditions .................................... 125

4.4.5 Solutions to Laplace’s Equation on Dielectric Boundaries ............ 126

4.5 Calculation of Electrostatic Loads ....................................... 127

4.6 Non-linear (NL) Integration scheme ..................................... 129

4.6.1 Newmark’s $\beta$ Equations: Implicit-Explicit Time integration ...... 130

4.6.2 NL Newmark Integration Scheme: Newton’s Method with Newmark’s $\beta$ equations ..................................................... 131

4.7 Verification of Developed FEM Model: Test Cases/Results .............. 133

4.7.1 Verification of The Electric Field ...................................... 133

4.7.2 Pull-in of Thin-film Electrostatically Actuated Fixed-fixed NEMS Switches with $g : l$ on the order of $10^{-3}$ ..................................................... 136

4.7.3 FEM Generated Detachment Curves .................................... 139

5 Design, Development, and Fabrication of WALD NEMS devices .......... 150

5.1 Overview ........................................................................ 150
5.2 Elementary Analytic Stress Analysis for Simple Devices .................................. 151
  5.2.1 Discussion ........................................................................................................... 152
5.3 1st Generation 2-terminal WALD NEMS Switches ............................................. 153
  5.3.1 1st Generation WALD NEMS Fabrication Process (50 nm gap-heights) 154
  5.3.2 1st Generation WALD NEMS 2-Terminal Fabrication Results ....... 155
5.4 FEM Stress Analysis and Re-design ........................................................................ 155
5.5 2nd Generation 2-Terminal WALD NEMS Switches (Entrenched Devices) .. 162
  5.5.1 2-Terminal WALD Entrenched NEMS Fabrication Process .......... 163
  5.5.2 2-Terminal WALD Entrenched NEMS Fabrication Results .......... 164
5.6 Entrenched 3-Terminal WALD NEMS Switches ................................................. 164
  5.6.1 Entrenched 3-Terminal WALD NEMS Fabrication Process .......... 167
  5.6.2 Entrenched 3-Terminal WALD NEMS Switches/Transistors Fabrication
      Results ..................................................................................................................... 168
5.7 Redesign of 3-terminal WALD NEMS Switches ................................................. 170
  5.7.1 Minimization of Over-etching and Associated Gate/Source Overlap . 171
  5.7.2 Characterization of Cavitation Effects .............................................................. 174
  5.7.3 Shorting Between Gate and Drain at Pull-in ..................................................... 175
  5.7.4 Redesigned 3-terminal WALD NEMS Switches and Fabrication Results 177
5.8 Design and Fabrication of Complementary WALD NEMS Inverters ............... 183
  5.8.1 Operating Principle ........................................................................................... 183
  5.8.2 FEM/FLFD Aided Design Study ....................................................................... 186
  5.8.3 Design and Fabrication of Bow-tie Shaped 3-terminal WALD NEMS
      Switches ................................................................................................................ 194
  5.8.4 Design of Poly-tie Shaped 3-terminal WALD NEMS Switches .......... 196

6 Characterization of WALD NEMS Devices ...................................................... 202
  6.1 Overview .............................................................................................................. 202
6.2 IV Characterization of Switching Behavior ................................................. 202
  6.2.1 1st Generation 2-terminal WALD NEMS Switches ............................. 202
  6.2.2 2nd Generation 2-terminal WALD NEMS Switches ............................. 205
  6.2.3 3-Terminal WALD NEMS Switches .................................................. 207
  6.2.4 Statistical Characterization of a 3-terminal WALD NEMS Switch ....... 209
  6.2.5 3-terminal WALD NEMS Switches with Wide Drains .......................... 214
  6.2.6 Gate-actuated Switching Behavior of 3-terminal WALD NEMS Switches/IV Characterization Setup Number 2 ........................................ 221
  6.2.7 3-terminal WALD NEMS Bow-tie Switches ....................................... 223
6.3 Dynamic Characterization of a 3-terminal WALD Switch: Switching Speed ................................................................. 228
6.4 Characterization of Tunneling Current for WALD NEMS Devices ............ 232
  6.4.1 Characterization of Tunneling Current Using STM theory ................... 232
  6.4.2 Characterization of Tunneling Using the Extended Field Emission Model 235
  6.4.3 % Difference Error in Characterization Introduced by a Linear Approximation ................................................................. 239
  6.4.4 Tunneling Conclusions .................................................................. 240
6.5 Reliability of WALD NEMS Devices ......................................................... 241
  6.5.1 1st Generation 2-terminal WALD NEMS Switches ............................. 241
  6.5.2 2nd Generation 2-terminal WALD NEMS Switches ............................. 241
  6.5.3 3-terminal WALD NEMS Switches .................................................. 242
  6.5.4 Reliability of 1st Generation WALD NEMS Tunneling Devices ........... 245
  6.5.5 Reliability of 2nd Generation 2-Terminal WALD NEMS Tunneling Devices ................................................................. 246
7 Conclusions/ Future Work ........................................................................ 260
  7.1 Dissertation Summary ........................................................................ 260
  7.1.1 List of Major Achievements ........................................................... 262
7.2 Envisioned Future Work .................................................. 264
   7.2.1 Devices ................................................................. 264
   7.2.2 Thermal Characterization of WALD Devices ................. 266
   7.2.3 WALD Material ...................................................... 266
   7.2.4 Device Physics ...................................................... 267
   7.2.5 Computational ...................................................... 268

Bibliography ........................................................................ 270

Appendix

A List of Symbols and Abbreviations ..................................... 287

B Irradiated CMOS ................................................................ 293
   B.1 CMOS Scaling ............................................................ 293
   B.2 Irradiation of MOS Devices ........................................ 296
      B.2.1 Radiation Induced Leakage Current and Carrier Mobility Degradation 302
   B.3 Micro to Nano Via Fabrication ..................................... 304
      B.3.1 Top-down and Pertinent Nano-capable Lithography Techniques ... 304
      B.3.2 Bottom-up ............................................................ 306
      B.3.3 Thin-film Sacrificial Layers ...................................... 307

C Approximation of Hamaker Constants via Lifshitz Theory .... 310
   C.1 Van der Waals Interaction and Hamaker Approximations via Lifshitz Theory 310
   C.2 Analytic Derivations for Different Material Systems Applicable to Thin-film
      NEMS devices .............................................................. 312
      C.2.1 Metal-Vacuum/Air-Metal ........................................ 312
      C.2.2 Metal-Vacuum/Air-Ceramic ...................................... 313
F.5.4 Displacement of Element Centers .......................... 383
F.5.5 Nodal Charge for Three-Terminal Devices .................... 383
F.5.6 Mechanical Boundary Conditions for Drain Electrode ............ 386
F.5.7 Electrostatic Domain Refinement to include Drain Geometry and Co-
ordinates .......................................................... 387
F.5.8 Drain Coordinate Transformation to Row and Column Space .... 392
F.5.9 Drain Coordinate Finder/Flagger .................................. 396
F.5.10 Coordinates of the Deformed Electrostatic Domain ............. 400
F.5.11 Electrostatic Force ............................................. 400
F.5.12 Mesh Refinement .................................................. 401
F.5.13 Gradient of the Potential for a Three-Terminal Device ....... 405
F.5.14 Pull-in Voltage .................................................... 409
F.5.15 Residual .......................................................... 412
F.5.16 Plotter ............................................................. 414
F.5.17 Load Interpolation from Electric to Mechanical Domain ....... 418
F.6 Utilities Specific to 2-Terminal Simulations ......................... 420
F.6.1 Elemental Capacitance for 2-Terminal Devices .................. 420
F.6.2 Nodal Charge for 2-Terminal Devices ............................ 420
F.6.3 Coordinates of Deformed Electrostatic Domain Field Points for a 2-
Terminal Device ...................................................... 421
F.6.4 Gradient of the Potential for a 2-Terminal Device ............... 422

G van der Waals Force Module ................................. 424
Tables

Table

3.1 Analytic Pull-in Voltages for Rectangular, Bow-tie, and 2nd order 2 and 3-terminal WALD NEMS switches ................................................................. 65
3.2 Tunneling model electric field study: $\beta$ Vs. Thin-film Thickness ........ 96
3.3 Tunneling model electric field study: $\alpha_1$ Vs. Thin-film Thickness .... 98
4.1 Comparison of FEM and Analytically Calculated Electric Field Values for 2 and 3-terminal Test Cases ................................................................. 136
4.2 Comparison of FEM and Analytically Calculated Pull-in Voltages for 2 and 3-terminal Test Cases ................................................................. 138
4.3 FEM and Analytically Calculated Critical Displacements for 2 and 3-terminal Test Cases ................................................................. 138
5.1 2-terminal WALD NEMS Switch Design: Fall 2008 .......................... 174
5.2 3-terminal WALD NEMS Switch Design: Spring 2009 .................. 175
5.3 3-terminal WALD NEMS Switch Design: Summer 2009 ............... 175
5.4 3-terminal Fixed-fixed WALD NEMS Switch Geometries (wide drain) .... 179
5.5 3-terminal Cantilever WALD NEMS Switch Geometries (wide drain) .... 181
5.6 CMEMS/NEMS inverter truth table ...................................................... 185
5.7 Poly-tie geometry/fitting parameters .................................................. 200
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>Pull-in and pull-out voltages from IV characterization of a 3-terminal WALD NEMS bow-tie switch</td>
<td>220</td>
</tr>
<tr>
<td>6.2</td>
<td>Pull-in and pull-out voltages from IV characterization of a 3-terminal WALD NEMS bow-tie switch</td>
<td>227</td>
</tr>
<tr>
<td>6.3</td>
<td>Dynamic response of a 3-terminal WALD NEMS switch</td>
<td>229</td>
</tr>
<tr>
<td>6.4</td>
<td>Summary of the theoretical and measured switching speeds of a WALD NEMS switch</td>
<td>231</td>
</tr>
<tr>
<td>6.5</td>
<td>Comparison of extracted barrier heights using linear and FEM approximated displacements for a 1st generation fixed-fixed 2-terminal WALD device</td>
<td>233</td>
</tr>
<tr>
<td>6.6</td>
<td>Comparison of extracted barrier heights using linear and FEM approximated displacements for a 2nd generation fixed-fixed 2-terminal WALD device</td>
<td>234</td>
</tr>
<tr>
<td>6.7</td>
<td>Fitting parameters used for tunneling current characterization of several WALD NEMS devices</td>
<td>237</td>
</tr>
<tr>
<td>6.8</td>
<td>% Difference Error in Tunneling Characterization Introduced by a Linear Approximation</td>
<td>239</td>
</tr>
<tr>
<td>6.9</td>
<td>Lock-in Amplifier settings for reliability characterization of WALD NEMS devices</td>
<td>244</td>
</tr>
<tr>
<td>A.1</td>
<td>List of symbols and abbreviations (A-E)</td>
<td>288</td>
</tr>
<tr>
<td>A.2</td>
<td>List of symbols and abbreviations (F-K)</td>
<td>289</td>
</tr>
<tr>
<td>A.3</td>
<td>List of symbols and abbreviations (L-R)</td>
<td>290</td>
</tr>
<tr>
<td>A.4</td>
<td>List of symbols and abbreviations (S-V)</td>
<td>291</td>
</tr>
<tr>
<td>A.5</td>
<td>List of symbols and abbreviations (W-Y)</td>
<td>292</td>
</tr>
<tr>
<td>E.1</td>
<td>FEM Model Units</td>
<td>324</td>
</tr>
<tr>
<td>E.2</td>
<td>Conversion Factors: Si $\rightarrow$ FEM</td>
<td>326</td>
</tr>
</tbody>
</table>
## Figures

**Figure**

2.1 Illustration of a binary ALD reaction ........................................ 10
2.2 Deposition of WALD monitored via QCM ................................. 10
2.3 Cross-sectional SEM image of 300 nm thick $\text{Al}_2\text{O}_3$ film deposited on Si wafer with trench structures. .............................. 11
2.4 Conformally coated ultrahigh-aspect-ratio nanopores ................. 11
2.5 SEM image of ALD Al2O3 micro-resonators .............................. 14
2.6 ALD alumina passive pointer test structure ............................ 15
2.7 MEMS microengine with a wear-resistant ALD Alumina coating ...... 16
2.8 Transmission electron microscopy image of a four-bilayer W/Al2O3 nanolaminate grown at 177 C ............................................ 17
2.9 Resistivity of WALD vs. Thickness ........................................... 18
2.10 Schematic representation of the WALD-coated Co nanoparticle with Co radius or layer thicknesses defined by $r_1$, $r_2$, $r_3$, and $r_4$ ......................... 19
2.11 1967 MEMS/MOS hybrid resonant gate transistor ..................... 20
2.12 MEMS resoswitch .............................................................. 22
2.13 A plastic MEMS switch ....................................................... 24
2.14 CNT NEMS tweezers .......................................................... 26
2.15 Vertically oriented 3-terminal CNT NEMS switches ................. 27
2.16 Three-terminal cantilever-type CNT NEMS switch ................. 28
2.17 Two-terminal CNT fabric based NEMS switch ........................................ 28
2.18 Two-terminal fixed-fixed SWNT NEMS switch .................................... 29
2.19 Two-terminal fixed-fied MWNT NEMS switch aligned via surface functional-
ization ........................................................................................................... 29
2.20 Laterally actuated TF NEMS switch ...................................................... 30
2.21 Cantilever based TF NEMS switch ....................................................... 30
2.22 Graphene breakjunction NEMS switch ................................................ 31
2.23 Graphene - $SiO_2$ Nanocable device .................................................... 32
2.24 CMOS/ CMEMS analog ........................................................................ 34
2.25 Polysilicon CMEMS inverter ................................................................. 35
2.26 Plastic CMEMS inverter fabricated using inkjet technologies ................. 36
2.27 Dynamic characterization of the plastic CMEMS inverter ................. 36
2.28 Schematic of a 4-terminal relay developed at Berkeley .......................... 37
2.29 4-terminal relay Waveform .................................................................. 38
2.30 Schematic of seesaw relay developed at Berkeley .................................. 39
2.31 Logic waveforms from the seesaw device developed at Berkeley .......... 42
2.32 SEM image of the SiC NEMS inverter developed at Case Western ........ 43
2.33 Waveform of a SiC NEMS inverter developed at Case Western ............. 43
3.1 Schematic of the Bow-tie structure as seen in the x-z plane ...................... 46
3.2 Schematic a general poly-tie structure as seen in the x-z plane ................ 46
3.3 General $\sigma - \epsilon$ curve for metal .......................................................... 48
3.4 A fixed-fixed beam subjected to a point load acting at some distance $a$ from
the left support, and the associated free-body diagram ............................... 50
3.5 Free-body diagram for $0 \leq x < a$ of a fixed-fixed beam subjected to a point
load acting at some distance $a$ from the left support ................................. 50
3.6  Free-body diagram for $a < x \leq L$ of a fixed-fixed beam subjected to a point load acting at some distance $a$ from the left support .......................... 50
3.7  Fixed-fixed beam subjected to a distributed load $\xi$ .......................... 53
3.8  Fixed-fixed beam subjected to a fully-distributed load ......................... 53
3.9  Fixed-fixed beam subjected to a centrally-distributed load ................... 59
3.10 A 2-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source ......................................................... 59
3.11 A 3-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source biased by $V_{DS}$ ......................................... 59
3.12 Fixed-fixed beam subjected to a bi-distributed load ............................ 60
3.13 A 3-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source, and geometrically symmetric, electrically connected gate electrodes biased by $V_{GS}$ ..................................................... 60
3.14 3-terminal Device schematic (x-y plane) ........................................ 63
3.15 Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices (rectangular profile) ......................................................... 63
3.16 Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices (bow-tie profile) ......................................................... 64
3.17 Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices ($2^{nd}$ order poly-tie profile) ........................................ 64
3.18 Comparison of Displacement Vs. Applied Voltage for 2-terminal WALD NEMS devices ................................................................. 66
3.19 Comparison of Displacement Vs. Applied Voltage for 3-terminal drain actuated WALD NEMS devices .............................................. 66
3.20 Comparison of Displacement Vs. Applied Voltage for 3-terminal gate actuated WALD NEMS devices .............................................. 67
3.21 Lumped sum model of MEMS/NEMS switch including van der Waals force . 69
xx
3.22 Variation of dimensionless parameter β with dimensionless parameter α . . .

73

3.23 Variation of pull-in gap uP I height with dimensionless parameter α . . . . .

73

3.24 Bifurcation diagram for Displacement Vs. β for varying values of α . . . . .

74

3.25 Bifurcation diagram for Displacement Vs. α for varying values of β . . . . .

74

3.26 Phase diagram of the system for α = α∗ and β = 0 . . . . . . . . . . . . . .

78

3.27 Phase diagram of the system for α = α∗ and β = 0.1 . . . . . . . . . . . . .

78

3.28 Phase diagram of the system for α = α∗ and β = 0.2 . . . . . . . . . . . . .

78

3.29 Phase diagram of the system for α = α∗ and β = 0.25 . . . . . . . . . . . . .

79

3.30 Phase diagram of the system for α = α∗ and β = 0 . . . . . . . . . . . . . .

81

3.31 Phase diagram of the system for α = α∗ and β = 0.1 . . . . . . . . . . . . .

82

3.32 Phase diagram of the system for α = α∗ and β = 0.25 . . . . . . . . . . . . .

82

3.33 Phase diagram of the system for α = α∗ and β = 0.25 . . . . . . . . . . . . .

83

3.34 Detachment length Vs. Initial Gap Height for representative fixed-fixed and
cantilever type NEMS systems . . . . . . . . . . . . . . . . . . . . . . . . . .

85

3.35 Model of an electron in a square well . . . . . . . . . . . . . . . . . . . . . .

87

3.36 Energy well for field emission . . . . . . . . . . . . . . . . . . . . . . . . . .

89

3.37 Illustration of a deflected fixed-fixed thin-film NEMS switch with cross-section 93
3.38 FEM calculated electric field around a rectangular conductor . . . . . . . . .

93

3.39 Electric-field study: EC Vs. Gap Height for varying thickness and applied
potentials . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

95

3.40 Electric-field study: β Vs. Thin-film Thickness . . . . . . . . . . . . . . . . .

96

3.41 Electric-field study: κ Vs. Applied Potential . . . . . . . . . . . . . . . . . .

97

3.42 Electric-field study: α1 Vs. Thin-film Thickness . . . . . . . . . . . . . . . .

97

3.43 Electric-field study: α1 Vs. Thin-film Thickness . . . . . . . . . . . . . . . .

98

3.44 Approximations of Displacement Vs. Applied Voltage . . . . . . . . . . . . . 101
3.45 Modeled Tunneling Current for a 2-Terminal WALD switch: 50 nm gap . . . 104
3.46 Modeled Tunneling Current for a 2-Terminal WALD switch: 15 nm gap . . . 105


3.47 Modeled Tunneling Current for a 2-Terminal WALD switch, FEM Vs. Linear Approximation: 50 nm gap

3.48 Modeled Tunneling Current for a 2-Terminal WALD switch, FEM Vs. Linear Approximation: 15 nm gap

3.49 Error between FEM and linear approximations: 50 nm gap

3.50 Error between FEM and linear approximations: 15 nm gap

4.1 General $\sigma - \epsilon$ curve for metal

4.2 Mapping of the FL mesh to some matrix A

4.3 FL nodal Nearest neighbor distances for an undeformed mesh

4.4 FL nodal nearest neighbor distances for a deformed mesh

4.5 FL nodal nearest neighbors in terms of forward and backward radii

4.6 Rectangular boundary illustrating boundary and corner cases for calculating average radial distances to nearest neighbors

4.7 Illustration of a simple rectangular electrostatic domain with Robin boundary conditions

4.8 Diagram illustrating parallel plate capacitance discretization parameter definitions

4.9 Diagram illustrating the tangential stiffness matrix and it’s role in Newton’s method

4.10 2-Terminal FEM Electrostatic Solution

4.11 3-Terminal FEM Electrostatic Solution

4.12 3-Terminal FEM Electrostatic Solution with $V_{DD} = V_{DS}$

4.13 2-terminal WALD NEMS Switch FEM Simulation

4.14 Drain Actuated 3-terminal WALD NEMS Switch FEM Simulation

4.15 Gate Actuated 3-terminal WALD NEMS Switch FEM Simulation

4.16 Drain Actuated 3-terminal WALD NEMS Bow-tie Switch FEM Simulation
4.17 Gate Actuated 3-terminal WALD NEMS Switch FEM Simulation  
4.18 Comparison of FEM and Theoretically Calculated Detachment Curves  
4.19 Bow-tie Detachment Study: Gap Height Vs. $W_M$ for Varying Lengths of 
WALD Bow-tie Structures  
4.20 Bow-tie Detachment Study: $\alpha$ Vs. Length and $\beta$ Vs. Length  
4.21 Detachment Curve for a WALD NEMS Bow-tie Device with Variation of $W_M$  
5.1 WALD NEMS Fabrication Process for 2-Terminal Devices with 50 nm Gaps  
5.2 Fabricated WALD NEMS Cantilevers/ 50 nm Gap  
5.3 Fabricated WALD NEMS Bridges/ 50 nm Gap  
5.4 FEM stress analysis of a 2000 x 700 x 30 nm WALD device  
5.5 FEM stress analysis of a 4000 x 500 x 30 nm WALD device  
5.6 FEM stress analysis for different WALD device geometries, and theoretical 
and experimental pull-in voltages (if available).  
5.7 Fabrication Process for 2nd generation 2-terminal WALD NEMS devices  
5.8 Fabrication results for 2-terminal WALD Trench Devices  
5.9 Fabrication process for 3-terminal Trench WALD NEMS switches  
5.10 3-D model and SEM images of 3-terminal WALD NEMS switch  
5.11 E-beam induced Cavitation  
5.12 IV curves demonstrating a short between drain and gate electrodes upon ac-
tuation  
5.13 FEM model demonstrated snap-through of device over a narrow drain electrode 
5.14 FEM model demonstrated snap-through of device over a wide drain electrode 
5.15 SEM image of a 3-terminal cantilever WALD NEMS switch that has failed 
because of welding  
5.16 Example of an e-beam mask file for a 3-terminal cantilever WALD NEMS device 
5.17 SEM images of a 3-terminal fixed-fixed WALD NEMS switch with wide drain
5.18 SEM images of a 3-terminal cantilever WALD NEMS switch with wide drain  
5.19 Circuit diagram for a CMEMS/NEMS inverter ........................................ 184 
5.20 Schematic of CMEMS/NEMS inverter operation ................................... 184 
5.21 SEM images of monolithically fabricated WALD CNEMS Inverters .............. 186 
5.22 FEM/FD Design Study for fixed-fixed CNEMS Inverters with rectangular 
profiles ........................................................................................................... 189 
5.23 .................................................................................................................. 191 
5.24 .................................................................................................................. 193 
5.25 FEM/FD Design Study for fixed-fixed CNEMS Inverters with bow-tie profiles 194 
5.26 Expected pull-in voltages for fabricated WALD NEMS bow-tie 3-terminal switch 195 
5.27 SEM images of 3-terminal bow-tie switches ............................................. 196 
5.28 FEM stress analysis of a bow-tie structure in tension ............................... 198 
5.29 FEM stress analysis of a poly-tie structure in tension ............................... 198 
5.30 Feasible design space for a 9th order WALD NEMS poly-tie 3-terminal device 199 
5.31 Schematic of a 9th order poly-tie WALD fixed-fixed beam ......................... 200 
5.32 Expected pull-in voltages for designed WALD NEMS poly-tie 3-terminal switch 201 

6.1 I-V curve for a WALD switch (50 nm Gen.) with current limited to 500 nA . 204 
6.2 Average pull-in and pull-out I-V curves over 5 cycles for a WALD (50 nm 
Gen.) switch with current limited to 100 nA .............................................. 204 
6.3 IV curves for 2-terminal WALD trench device taken at 1 atm and 30 mTorr; 
various current limits ...................................................................................... 207 
6.4 IV curve comparison, 1 atm Vs. 30 mTorr; current limited at 500 nA ...... 208 
6.5 IV characterization of a 3-Terminal WALD NEMS Switch ......................... 211 
6.6 Comparison of the average IV curves for a 3-terminal WALD NEMS switch 
for $V_{GS} = 0$ and 2 Volts .............................................................................. 213
6.7 Plot of average pull-in voltages for statistical IV characterization of 3-terminal WALD NEMS switch .................................................. 214
6.8 Tukey’s comparison of average pull-in voltages for a 3-terminal WALD NEMS switch .................................................................................. 215
6.9 .......................................................................................................................................................................................... 215
6.10 IV curve showing common shorting of 3-terminal WALD NEMS switches with narrow drains ........................................................................................................ 216
6.11 IV curves for a fixed-fixed 3-terminal WALD switch \((D_W = 2 \text{ um})\) .................................................................................................................................. 217
6.12 IV curves for a cantilever 3-terminal WALD switch \((D_W = 2 \text{ um})\) ......................................................................................................................... 219
6.13 Measured Hysteresis of Pull-in/out Switching Behavior for a 3-terminal WALD NEMS Device .................................................................................. 220
6.14 Circuit diagram for experimental IV setup .......................................................................................................................... 222
6.15 IV curve for drain-actuated switching of a 3-terminal WALD NEMS switch ...................................................................................... 224
6.16 IV curve for gate-actuated switching .......................................................................................................................... 224
6.17 .......................................................................................................................................................................................... 225
6.18 IV curve for gate-actuated switching of a 3-terminal WALD NEMS bow-tie switch: \(V_{DD} = 0.075, 0.1 \text{ V}\) ................................................................................................................................ 247
6.19 IV curve for gate-actuated switching of a 3-terminal WALD NEMS bow-tie switch: \(V_{DD} = 0.25, 1 \text{ V}\) ................................................................................................................................ 248
6.20 Pull-in/out voltage Vs. \(V_{DD}\) for a 3-terminal WALD NEMS bow-tie switch .................................................................................. 249
6.21 Circuit diagram for impulse response characterization apparatus .......................................................................................... 249
6.22 Square wave response of a drain-actuated 3-terminal WALD NEMS switch .................................................................................. 250
6.23 Measured IV curves taken before and after the impulse response experiment .................................................................................. 250
6.24 1\textsuperscript{st} generation fixed-fixed 2-terminal WALD device tunneling IV curves .................................................................................. 251
6.25 Semi-log plot of tunneling current for a 1\textsuperscript{st} generation fixed-fixed 2-terminal WALD device .................................................................................. 252
6.26 Comparison of extracted barrier heights using linear and FEM approximated
displacements for a 2\textsuperscript{nd} generation 2-terminal WALD device .......... 252
6.27 Extended tunneling model fit to the IV curve of a fixed-fixed 2\textsuperscript{nd} generation
2-terminal WALD switch ....................................................... 253
6.28 Extended tunneling model fit to the IV curves of a fixed-fixed 2\textsuperscript{nd} generation
2-terminal WALD switch taken at 1 atm and 30 mTorr .......................... 253
6.29 Extended tunneling model fit to the IV curve of a fixed-fixed 3-terminal WALD
switch .......................................................... 254
6.30 Extended tunneling model fit to the IV curve of a fixed-fixed 3-terminal WALD
bow-tie switch .......................................................... 255
6.31 Extended tunneling model fit to the IV curve of a fixed-fixed 2\textsuperscript{nd} generation
2-terminal WALD switch via a linear approximation .......................... 256
6.32 Extended tunneling model fit to the IV curves of a fixed-fixed 2\textsuperscript{nd} generation 2-
terminal WALD switch taken at 1 atm and 30 mTorr via a linear approximation 256
6.33 Circuit diagram for low-frequency reliability characterization experimental setup 257
6.34 Actuation until failure of a 3-terminal WALD NEMS switch ............... 258
6.35 IV curve of lifetime testing for a doubly clamped device shown to have a
lifetime > 660,500 cycles .................................................. 259

B.1 An NMOS transistor in the off-state ........................................ 294
B.2 CMOS transistor cross-section ............................................. 294
B.3 Schematic of n-channel MOSFET illustrating radiation-induced charging of
the gate oxide .......................................................... 297
B.4 Schematic illustration of the LOCOS field oxide isolation structure and pos-
sible leakage paths ...................................................... 298
B.5 Schematic illustration of the I-V characteristic of an n-channel gate oxide
transistor before and after irradiation ...................................... 299
B.6 Positive charges trapped in the spacers and its effects for NMOSFETs and PMOSFETs ........................................ 300
B.7 $I_{ds} - V_{ds}$ characteristics before and after protons exposure $1 \times 10^{15}$ protons/cm$^2$ for NMOSFETs and PMOSFETs .... 300
B.8 $I_{ds} - V_{gs}$ and $g_m - V_{gs}$ characteristics ($V_{ds} = 0.05V$) before and after proton exposure for NMOSFETs and PMOSFETs ....... 301
B.9 Gate currents in the RILC regime after a 5.3 Mrad(Si) gamma dose for N/P-MOS devices ............................................ 303
B.10 Fabrication technique and their dimensional limits .......................................................... 306
D.1 Structures used for cavitation/RIE characterization ..................................................... 317
D.2 Comparison of the narrowest rectangular structures etched in RIE for 70 and 136 seconds before metal deposition/lift-off .............. 318
D.3 SEM images illustrating how the rectangular structures merge as a result of cavitation/RIE .................................................. 318
D.4 Average over-etch width Vs. designed width ................................................................. 320
D.5 Average over-etch rate Vs. designed width ................................................................. 320
D.6 Average over-etch rate for structures etched for 70 and 136 seconds ......................... 321
D.7 SEM images of 3-terminal Poly-tie switches with overlapping gates .......................... 321
D.8 SEM images of merged gate electrodes, and un-merged gate electrodes ................. 322
E.1 FEM Model Structure for Self-consistent Solutions .................................................. 325
Chapter 1

Introduction

1.1 Motivation

Complementary metal-oxide-semiconductor (CMOS) integrated circuit (IC) technology permeates our daily existence. Although CMOS technology was invented in 1963, it was not widely adopted to very-large-scale-integration (VLSI) chips until the 1980’s. The shift was a result of the power crisis in the 1980’s. Until that point NMOS had been the dominant transistor technology used in VLSI chips, but because CMOS processors only used roughly a tenth the power of a similar NMOS processor, CMOS became the standard in transistor technology [93]. The technology has profoundly affected our lives, from the way we work, learn, communicate, and entertain ourselves, to the way that we procure food. In fact, one could easily make the argument that CMOS technology has largely been responsible for setting the trajectory of our continually evolving culture for the past 30 years.

Gordon Moore, one of the founders of Intel, observed in the early 1970’s that the number of transistors per chip had been increasing at an exponential rate for several years. He predicted that the transistor count in state-of-the art processors would double every 18 months – this has come to be known as Moore’s law [24]. The continual scaling of CMOS technology with every design node has persisted according to Moores law for the last 40 years; however, in the past decade the continued scaling of transistor dimensions in CMOS technology reached a physical material limit, which resulted in a massive increase in power dissipation – the sum of both increased dynamic power dissipation and sub-threshold leakage
currents. An unacceptably large percentage of the power dissipated was due to the massive increase in sub-threshold leakage current, which is a direct consequence of the material limit reached via scaling. Thus while the number of transistors continued to double as predicted by Moore’s law, the new technology progressed at the expense of power efficiency. Further scaling of the existing technology, if possible, could only be accomplished at the expense of device performance.

The nearly complete integration of CMOS technology into consumer products has been a monumental achievement; however, as we continue to explore our universe with the aid of scientific instruments (both on earth and in space) the radiation sensitivity, and the limited-temperature functionality of CMOS technologies, become progression limiting factors. CMOS materials are sensitive to temperature variations, which affect carrier concentrations and mobility [33], as well as low doses of radiation, such as that of alpha decay, which is known to be responsible for soft error in memory devices [213, 207, 239]. Radiation-hard devices make up a large segment of the aerospace/military integrated circuit market, with an increasing importance for space applications. The overall reliability and performance of IC technologies is becoming increasingly important, as the space community has begun to adopt a more commercially off-the-shelf approach, implying the need for more advanced materials and components [86].

1.2 Scope and Application

As micro-chips are increasingly used in portable consumer electronics the need to develop low power circuits becomes crucial; that is, the overall power used by the integrated circuit must be kept at a minimum. In a cellular phone for example, existing transistors consume milli-watts of power continuously, thereby draining the battery, whereas capacitive micro-switches consume power only during actuation [94], thus the integration of MEMS/NEMS mechanical switches, and/or transistors, offers an attractive avenue in the quest to reduce power consumption. Power dissipation presents a serious problem because increased
power consumption and its subsequent, and necessary, heat removal limits integration possibilities in current CMOS technologies. One possible solution to this power dissipation problem lies in the development of CMOS integrable nano-electromechanical (NEMS) switches for the development of hybrid NEMS/CMOS systems.

There are several exciting applications of CMOS compatible NEMS switches. Because leakage current in a NEMS switch is limited to Brownian motion [34] and tunneling current, the total leakage current should nearly be eliminated. Therefore as IC technologies continue to scale, the integration of NEMS devices as physical switches between transistors and their circuits, or larger components of the circuit, such as blocks of RAM, represent a feasible and novel solution to help mitigate the increasing power demands of next generation technologies.

In addition to power savings applications, and perhaps even more exciting, NEMS switches offer the possibility of developing entirely mechanical microcontrollers/microprocessors capable of operating in high-temperature and/or irradiated environments not accessible to tradition electronics. Currently high temperature (300-900 C) operation is not possible with state-of-the-art semiconductor processes because conventional electronics fail at approximately 300 C [27], but NEMS devices fabricated with refractory materials, or other materials capable of high-temperature operation such as silicon carbide, which is a wide band gap semiconductor [40], could be designed to operate at extremely high temperatures. Furthermore, unlike MOS components, the performance of conductor based capacitive MEMS/NEMS devices should not be susceptible to radiation effects. At most, in a metal radiation may introduce point defects in the crystal lattice, which may act as scattering centers, thereby reducing electron mobility and increasing the overall resistivity of the material. However, even if the device were irradiated by such high doses of radiation as to cause significant damage to the crystal lattice of the conducting material, the device would not lose its ability to store charge, and therefore would continue to operate as designed. Therefore conductor-based electrostatically actuated MEMS/NEMS devices should be largely impervious to the damaging effects of radiation that hinder the use of MOS devices in low-to-hard radiation
environments.

The majority of NEMS switches to date have been based on carbon-nano-tube (CNT) designs. The devices consume little power during actuation, and as expected, have demonstrated actuation voltages much smaller than MEMS switches. Unfortunately, NEMS CNT switches are not typically CMOS integrable due to the high temperatures required for their growth, and their fabrication typically results in extremely low and unpredictable yields.

More recently an increasing effort has been put forth in the study and development of thin-film based NEMS capacitive switches. This effort includes my own and serves as the central focus of my proposed dissertation. Thin-film NEMS devices offer great advantages over more commonplace CNT devices for several reasons, including: higher fabrication yields, low-temperature (CMOS compatible) deposition techniques such as ALD, and increased control over design parameters/device performance metrics, i.e., device geometry. Furthermore, as will be seen in chapter 5, top-down, thin-film, nano-fabrication techniques are better capable of producing complicated device geometries than CNT based processes, enabling the design and development of multi-terminal switches well-suited for low-power hybrid NEMS/CMOS systems as well as complementary-biased electromechanical switches for the construction of NEMS inverters, the use of which should be well suited to temperature/radiation hard computing architectures.

1.3 Achievements

The primary focus of this research has been the development of atomic layer deposition (ALD) enabled NEMS switches and logic devices. The devices developed here were fabricated via a novel, top-down, low-temperature, and CMOS integrable technology, using for the first time ALD tungsten (WALD) as the primary structural material in a MEMS or NEMS device. The major achievements of the research effort summarized in this dissertation include:
1. During the course of this research two different novel, top-down, low-temperature, CMOS integrable fabrication technologies, employing WALD as a structural layer for MEMS or NEMS devices, were developed. The fabrication processes developed are robust yet simple and capable of producing a wide array of novel NEMS devices. The developed fabrication processes build upon traditional micro-machining techniques and introduce new methods specifically suited for NEMS thin-film devices, thereby expanding the possibility of future fabrication technologies and associated devices.

2. Using the developed fabrication technologies, several generations of WALD NEMS switches were successfully designed, fabricated, and characterized. Previously, ALD materials had been used primarily as protective coatings, or hydrophilic/hydrophobic coatings, but here for the first time an ALD material was successfully integrated into a nano-scale fabrication process as the structural material for an electrostatically actuated device. The ultra-thin films allowed for the fabrication of devices with very low, CMOS compatible actuation voltages. Characterization of the WALD switches developed here demonstrated functionality in a low-current tunneling regime. Thus the devices have the potential to be used as the building blocks for novel devices not possible using traditional CMOS technology, i.e., high-density tunneling logic devices.

Demonstrated WALD NEMS switches include:

* 2-terminal, surface micromachined WALD NEMS fixed-fixed and cantilever switches having gate-to-source gap heights of 50 nm

* 2-terminal, entrenched WALD NEMS fixed-fixed switches having gate-to-source gap heights of 30 nm

* 3-terminal, entrenched WALD NEMS fixed-fixed and cantilever switches having gate-to-source gap heights of 50-65 nm, and drain-to-source gap heights of 20 nm
* 3-terminal, entrenched WALD NEMS fixed-fixed bow-tie and ninth-order poly-tie switches having gate-to-source gap heights of 50-65 nm, and drain-to-source gap heights of 20 nm

3. A FEM/FD based multi-physics model for 2 or 3-terminal devices whose electrostatic domain has an aspect ratio on the order of $10^{-3}$ was developed. The model uses a faux-Lagrangian mesh finite difference method to solve the Potential problem (Laplace’s Equation) for a quasi-statically deforming domain. The approach developed here allows for the study and numerical characterization of thin-film NEMS device designs which are not feasible using a commercially typical non-specialized FEM/BEM approach. Using the FEM/FD based numerical model, coupled with the extended tunneling model, the characterization of the tunneling regime has been improved. Furthermore, the development of this model allowed for the discovery of CNEMS Inverter design rules specific to ultra-thin film NEMS devices similar to those developed by this research effort.

1.4 Organization of Dissertation

The general motivation and achievements of this research have been presented. The remainder of this thesis has been organized into chapters of pertinent information. The second chapter presents a focused literature review of topics critical to the proposed research. These topics include: a brief introduction to ALD, WALD uses to date, a review of MEMS/NEMS capacitive switches including the current state-of-the-art, and finally a review of MEMS/NEMS logic devices similar to those studied/proposed here.

The third and fourth chapters are devoted to modeling that is relevant to the devices developed herein, as well as similar thin-film NEMS devices and any devices that may be designed using the ALD thin-film fabrication processes developed in this thesis. Chapter three focuses particularly on analytic modeling, while chapter four focuses on the development of a
FEM/FD Multi-Physics model for 2 or 3-terminal thin-film electrostatically actuated NEMS switches. The model was specifically developed for devices whose electrostatic domain has aspect ratios on the order of $\approx 10^{-3}$, for which solutions via commercial software are difficult to resolve.

In chapter three the reader will find the derivation of analytic formulas for the calculation of effective stiffness for fixed-fixed beams with symmetric, non-rectangular profiles subject to partially distributed loads. These formulas are then applied to the standard 1-D lumped model for calculating the pull-in as a function of gap-height. The middle of the chapter is devoted to van der Waals interactions for different material systems and to the effect of the interaction on system dynamics and stability. The chapter concludes with a tunneling current model better suited for application to MEMS/NEMS switches than what is commonly reported in literature.

As already mentioned, chapter four is devoted entirely to the development of a FEM/FLFD Multi-Physics model for 2 or 3-terminal thin-film electrostatically actuated NEMS switches. In this chapter the derivation of a finite element model for the mechanical domain is presented in some detail, followed by the derivation of the faux-Lagrangian mesh, the finite-difference method for the solution of Laplace’s equation which describes the electrostatic domain. After the physical models have been discussed, the non-linear numerical solver employed to solve the electromechanical system at some time-step $t^k$ is presented in detail. Finally, the self-consistent algorithm used for quasi-static analysis of the electromechanical system is given, followed by the results of specific case studies used as a check of model adequacy.

In the fifth and sixth chapters a comprehensive summary of the devices developed by this work is given. The summary chronicles the design, fabrication, and characterization of WALD NEMS 2-Terminal switches, 3-Terminal Switches and WALD CNEMS inverters. Chapter five focuses on the design and development of WALD NEMS 2-Terminal switches, 3-Terminal Switches, and WALD CNEMS inverters and their associated fabrication processes. Chapter six summarizes the characterization of the developed devices. In this chapter the IV
characterization/pull-in voltages for all of the switches developed are given, tunneling current measurements are presented, and results from switching lifetime tests for 2 and 3-terminal switches reported.

Finally, the seventh chapter concludes this dissertation. Here the reader will find a summary of the achievements of this research and a discussion of significant contributions to the field of NEMS. Finally, a brief summary of possible subsequent and relevant work extending from, or related to, the work encompassed by this thesis is given.
Chapter 2

Literature Review and the State-of-the-art

2.1 ALD

Atomic layer deposition (ALD), also known as atomic layer epitaxy (ALE) [187], is a thin film deposition technique that produces accurately controlled, dense inorganic films at low processing temperatures. ALD is a CVD-based process, based on the sequential repetition of self-limiting surface reactions: $A + B \rightarrow C + D$ [83]. For all ALD processes the two reactants, A and B, are applied in a binary sequence, i.e., ABAB..., thus obtaining precise, atomic-level control over deposition thickness [73, 137, 187], figure 2.1. Each half-reaction involves a reaction between a gas-phase precursor and a surface functional group. The surface reaction continues until all functional groups have been consumed and replaced with a new functional group [194, 195]. Figure 2.2 clearly illustrates the introduction of reagents and subsequent self limiting reaction/ material deposition for WALD.

Furthermore, ALD films are pinhole free, and can be grown with accurate control in high to ultra-high aspect ratio structures, making them ideal for coating applications in the MEMS/NEMS and IC industries [62, 81, 187]. Figure 2.3 shows high-aspect ratio trenches etched in Si conformally coated by ALD $Al_2O_3$ and TiN [187], and figure 2.4 shows ultrahigh-aspect-ratio nanopores ($1/d = 10^3$) conformally coated by ALD $Al_2O_3$ and $ZnO$ [66].

A great number of materials can be grown via ALD. Because of its binary reaction sequence, ALD easily facilitates the growth of compounds, thus the majority of ALD materials
Figure 2.1: Illustration of a binary ALD reaction [92]

Figure 2.2: Deposition of WALD monitored via QCM

consist of dielectrics such as $Al_2O_3$, $TiO_2$, or $HfO_2$ to name a few [112, 83, 25]; however, there also exist a number of single-element ALD materials such as: ruthenium, platinum,
Figure 2.3: Representative cross-sectional SEM image of 300 nm thick $Al_2O_3$ film deposited on Si wafers with trench structures. [187]

Figure 2.4: SEM images of uncoated anodic alumina membrane: a) cross-sectional view of 40-nm diameter pores; b) top view of hexagonal pore array [66]

iridium, rhodium, palladium, and tungsten [2, 4, 3, 83]. These single element ALD materials have applications in IC technology, as gates, interconnects, diffusion barriers [215] or seed
layers [2, 4]. However, because of its high melting temperature, stiffness [33], demonstrated toughness [149], and CMOS compatibility [149], WALD represents an excellent choice for the structural material in the development of novel CMOS compatible NEMS devices for use as mechanical switches, transistors, logic, or non-volatile memories, all capable of reliable performance in harsh environments.

2.1.1 WALD

WALD is a single-element ALD process based on the sequential exposures of $WF_6$ and $Si_2H_6$, whose chemistry has been thoroughly studied and growth precisely characterized [194, 195, 123, 82, 229]. The WALD deposition processes has been thoroughly studied and confirmed by a number of authors using several different techniques including: quadropole mass spectrometry [83], auger electron spectroscopy (AES) [64, 63], x-ray photoemission spectroscopy (XPS) [233], spectroscopic ellipsometry, Fourier transform infrared vibrational spectroscopy (FTIR) [223, 127, 126, 122, 123], and in-situ quartz crystal microbalance (QCM) [216]. In 2004 Grubbs et al. conducted a detailed study of the stoichiometry of the WALD reaction process at 200 C [83]. The proposed binary reaction sequence for WALD is given by equations 2.1-2.3.

$$WSiHFSiH_3^* + 2WF_6 \rightarrow WWWF_4^* + 2SiF_4 + \frac{3}{2}H_2 + HF$$ (2.1)

$$WF_4^* + Si_2H_6 \rightarrow WSiH_2F^* + SiHF_3 + \frac{3}{2}H_2$$ (2.2)

$$WSiH_2F^* + \frac{1}{2}Si_2H_6 \rightarrow WSiHFSiH_3^* + \frac{1}{2}H_2$$ (2.3)

In the given reaction process $X^*$ represents a surface species. From the reaction process it is seen that WALD film growth is achieved following the sacrificial reaction of disilane. The sacrificial disilane reaction occurs by an initial reaction of $Si_2H_6$ with $WF_4^*$ surface species.
to yield a $WSiH_2F$ surface species, equation 2.2. In the subsequent reaction, equation 2.3, $Si_2H_6$ undergoes bond insertion in SiH bonds [216]. The process is repeated until a desired thickness of WALD has been achieved.

2.1.2 ALD use in MEMS and NEMS to Date

To date ALD thin films have had limited use in the fabrication of MEMS or NEMS devices. ALD $Al_2O_3$ has been used as a micro-/nano-scale structural material [38, 217, 218] and as a protective and wear resistant coating for MEMS devices [92, 157]. Chang et al. used ALD alumina as the structural material for micro-resonators. The resonating structures were actuated electrostatically and resonant modes detected via laser interferometry. After measuring the resonant modes of their devices Chang et al. were able to successfully determine the residual stress in the ALD alumina film. The resonating structures fabricated by Chang et al. are shown in figure 2.5 [38].

Tripp et al. previously used ALD alumina in the fabrication of deformable membranes for adaptive optics. Large deformable membranes were fabricated using SOIMUMPS in conjunction with ALD and assembled using the flip chip bonding technique [217]. The membranes had a working area of 2 mm with a thickness of only 30 nm, and were coated by 4 nm of a sputtered Au-Pd alloy to allow for electrostatic actuation. Tripp et al. also used ALD alumina to fabricate passive micro test structures that were used to characterize the residual stress and mechanical properties of the ALD film [218]. Using these devices Tripp et al. found ALD alumina to have a Youngs modulus in the range of 168-182 GPa, a Berkovitch hardness of 12.3 GPa, a universal hardness of 8GPa, and the intrinsic in-plane stress in the range of 383-474 MPa. A passive pointer structure used by Tripp et al. to study residual stress is shown in figure 2.6.

To date the majority of research into ALD applications has been in thin film coating technologies. Work has been done on wear resistant coatings [157], creep suppression coatings [240], generally protective coatings [92], and hydrophobic coatings [89]. Mayer et al.
demonstrated the use of ALD $Al_2O_3$ as a wear resistant coating for a MEMS micro-engine. The group coated a MEMS micro-engine with a 10 nm thick layer of ALD Alumina, successfully demonstrating the ability of ALD to coat high aspect ratio surfaces as well as shadow regions, shown in figure 2.7. Mayer et al. demonstrated that by coating a device in ALD alumina, less wear particles were generated when compared to the same device coated only by native oxide, thus demonstrating ALD alumina’s utility as a wear resistant coating [157].

Another interesting avenue of research has been into the development of ALD nanolaminates with tailored physical properties. Physical properties far more exotic than those seen in bulk materials can be achieved when nanolayer thicknesses are less than the length scale that governs the physical property [193]. Work has been done on high-k nanolaminate dielectrics that can withstand very large electric-fields, are thermally stable, have superior insulation properties, far superior to bulk dielectrics, and demonstrate engineer-able leakage
Figure 2.6: a) A schematic of a pointer test structure, b) close up micrograph of a displaced pointer tip [218]

... currents [163, 131, 130, 65], as well as W/alumina nanolaminates with novel properties, such as increased hardness and ultra-low thermal conductivity, figure 2.8 [193, 45].

2.1.3 W use in MEMS/NEMS

WALD has tremendous potential for use in IC applications such as contact hole filling for source, drain, and gate metallization in MOSFETs [121], because W makes an ohmic
Figure 2.7: a) MEMS microengine, consisting of a gear turning on a hub. The structure uses 3-mm-thick polycrystalline Si for mechanical structures. The sacrificial oxide has been removed to release the device. b) Cross section of the hub showing the contact surfaces of the gear and hub, and the buried channel in the interior of the hub [157].

Contact with semiconductors and makes an effective diffusion barrier [189, 215]. As such, the electrical properties of WALD have been thoroughly studied [227, 121]. Kim et al. found that the resistivity of WALD films increases as the film thickness decreases, figure 2.10. Compared to CVD W all of the WALD thin films studied showed high resistivities (125-145 $\mu\Omega$-cm) for a thickness of $\sim$20 nm. By comparison, the resistivity of CVD W with a thickness of $\sim$18 nm has been measured to be $\sim$25 $\mu\Omega$-cm. Wilson et al. measured a resistivity of 100-400 $\mu\Omega$-cm for WALD films with a film thickness of 95-845 Å, confirming the findings of Kim [227]. It is thought that Si impurities, which introduce electron scattering cites, are responsible for the higher resistivity [189, 120].

Tungsten has seen very little use in MEMS applications. To date tungsten's use has
been limited to a wear protection coating (CVD) [149] and as a multilayer coating for x-ray reflectivity enhancement of polysilicon micro-mirrors [216]. Mani et al. deposited a 15 nm thick layer of CVD W on a MEMS micro-engine for use as a wear protection coating. The W coating provided a dramatic improvement in the wear characteristics of the device. The micro-engine devices coated by CVD W were observed to fail after a mean of $2 \times 10^6$ cycles with one device operating normally for more than $10^9$ cycles, a vast improvement over the uncoated devices which had a median lifetime of $4 \times 10^5$ cycles. Furthermore, FIB cross-sections of the coated micro-engines reveled no wear particle generation in the hub or near
the pin joint of the device.

More recently, Wilson et al. used WALD to coat cobalt nano-particles, figure 2.10. It was found that the properties and reactivity of nano-particles can be tuned by depositing thin coatings on their surfaces, thereby altering the surface-to-volume ratio as well as the surface energy of the particle. During this study native $WO_3$ formation was also studied, and it was discovered that the native oxide thickness is dependent on local curvature [228].

As a structural material in MEMS or NEMS, WALD has seen no use to date apart from the recent work presented in chapters 5 and 6, and references [54, 52, 195, 194]. Furthermore because little work has been done on the integration of WALD as a MEMS/NEMS capable structural material, no work has been done to study the mechanical/ thermomechanical properties of WALD. Thus far it has been assumed by us, in the design of our electrostatically actuated NEMS devices, that the Youngs modulus of WALD is the same as that of bulk W. This may be a reasonable assumption seeing that unlike ALD ceramics such as alumina,
which are amorphous and exhibit stiffness lower than their bulk counterparts [218], WALD films are known to possess a mixture of nano-crystalline alpha and beta-phase crystalline structures with grain sizes ranging from 9-17 nm [121] and have the same density as bulk W.

2.2 Electrostatic Micro/Nano Mechanical Switches and Logic Devices

2.2.1 MEMS Switches

Micromechanical switches were first demonstrated in 1971 [180] as electrostatically actuated cantilever switches used to switch low-frequency electrical signals, but may have been first proposed in the mid to late 1960s. Nathanson had developed suspended gate FETs,
what might be considered some of the first MEMS/MOS hybrid devices, by 1966 [169], and in his 1967 paper described the pull-in phenomena both conceptually and mathematically for cantilever beams [170]. However, Nathanson’s devices were not intended for switching purposes. Instead his suspended gate FETs were used as novel Q-tunable frequency filters [169, 170, 179]. Nathanson’s suspended cantilever FET device is shown in figure 2.11.

![Figure 2.11: Schematic of Nathanson’s 1967 resonant gate transistor for Q-tunable frequency filters [170]](image)

In the 1970s Preston, and Cosentino and Stewart, studied the electrostatic deflection of thin-film metal sheets suspended 5 um above the substrate on support structures[179]. This
work influenced the work of Petersen [179, 180], who in 1978 fabricated and tested MEMS capacitive cantilever switches for use in light modulation. Petersen’s devices were fabricated by patterning SiO$_2$ structures, coating them in a conductive layer of Cr/Au, and then suspending them via an EDP etch of the 100-oriented Si substrate. Those cantilever’s actuation voltages were in the range of 60-70 Volts, a value competitive with most devices through the 1990s [refs, [143]], and demonstrated lifetimes in excess of $10^6$ cycles. Furthermore, in his 1978 paper Petersen proposed that micromechanical devices should be integrated with IC processing techniques for the creation of novel MOS systems, just as we propose to do today using NEMS devices [179].

While some of the distinct advantages of MEMS switches were recognized in the 1970s, namely: extremely high off-state to on-state impedance ratios, high device densities, very low off-state capacitive coupling between contacts, and very low switching and sustaining powers, their research and development did not fully take off until the early 1990s. Petersen was awarded a US patent for a passive MEMS switch in 1985 [181], but research efforts really began when Larson, working Hughes Aircraft Company in Los Angeles, filed a US patent request for a rotary based electrostatically actuated MEMS switch [132].

MEMS switches developed to date have been fabricated using a variety of fabrication techniques, from bulk micromachining to surface micromachining, and combinations thereof, and have employed the use of numerous materials, such as semi-conductors, metal-coated dielectrics, and metals. The devices have been developed using a host of different and novel designs, from rotary switches, sliding switches, and lateral switches, to more traditional suspended bridge-type designs. Most importantly though, micromechanical switches have shown their utility in a number of different applications, such as: optical switching, light modulation, phase shifting, RF switching, and relay switching [36]. Because RF MEMS switches out-perform PIN diode and FETs in terms of insertion loss, isolation, and switching figure of merit (FOM) which defined as the product of capacitance and resistance, the most successful applications for MEMS capacitive switches have been in RF devices. Unfor-
Fortunately, the slower switching speeds (1-15 ns versus 0.16-1 ns for FETS) and lower lifetimes of RF MEMS devices (on the order of 100 billions cycles for FETS) typically limit their use to antenna switching, reconfigurable aperture, and instrumentation switching applications [143]. Furthermore, RF MEMS switches are typically constrained to actuation voltages of ~50 V because of competitive limitations regarding off-state isolation, FOM, restoring force, and thus associated reliability [143].

2.2.2 MEMS State-Of-The-Art Electrostatically Actuated Switches

Lin and Nguyen at Berkeley have recently developed the MEMS resoswitch, figure 2.12. The device exploits the resonance and nonlinear dynamic properties of its mechanical structure to greatly increase the switching speed and lifetime, while lowering the required actuation voltage, all by a substantial margin when compared to existing RF switches. The device is a disk resonator that is operated via a 2.5 Volt amplitude AC signal at frequency of 61 MHz, the resonant frequency of the disk. As the device resonates, it impacts electrodes along its orthogonal axis, thereby closing the switch. The device has an effective rise time less than 4 ns, more than 200 times faster than the fastest RF MEMS devices, and has been observed to operate for more than 16.5 trillion cycles. The MEMS resoswitch shows great promise for use in switched-mode power converters and power amplifiers [143].

Figure 2.12: SEM of the polysilicon MEMS resoswitch recently developed at Berkeley [143]
While the resoswitch represents the state-of-the-art in RF MEMS switches regarding operation and performance, MEMS switches developed by Nakano and Yokota et al. represent the state-of-the-art in micro-fabrication techniques. Their research group has successfully designed, fabricated, and demonstrated MEMS cantilever switches fabricated using inkjet-printing technology [167, 236]. Playing off of the current interest in flexible electronics the group has developed plastic MEMS switches applied to a wireless power transmission sheet. The devices are fabricated by adhering two 50 $\mu$m polyimide sheets together which have had control and signal electrodes printed on them using an inkjet printing machine with silver nanoparticles. The fabricated cantilevers have dimensions of 6 x 4.5 x 0.05 mm$^2$, with nominal gap heights of 50 $\mu$m. The operating voltage of the devices was measured to be 6.6 Volts, which is much less than typical MEMS switches, and comparable to some NEMS switches [9, 61, 101, 117, 119, 140, 204]. Finally, the devices have demonstrated lifetimes greater than 2 million cycles with little change in contact resistance indicating their long-term reliability [167]. An illustration of the cross-section and a photograph of the plastic MEMS device are shown in figure 2.13.

2.2.3 NEMS

The past 20 years have seen the rapid growth in MEMS from a field of novel research to a consumer market. Today MEMS devices are commonplace in a range of products, from cars, to watches, phones, and video game controllers. In the past decade or so, because of the continual effort to further miniaturize micro-mechanical devices, the field of MEMS has branched into a very active field of research in NEMS. The transition from MEMS to NEMS enables us to take advantage of the superior properties of nanomechanical systems, including: high natural frequencies, low mass, and ultra-low power consumption. Because NEMS switches have a much higher natural frequency than their MEMS counterparts, and thus a faster switching time, NEMS switches can be utilized as traditional electrical components, such as: transistors, amplifiers, adjustable diodes, inverters, memory cells, pulse position
modulators, variable resistors, switching systems, and phase shifters [183] – to name a few.

2.2.4 Carbon Nano-tube (CNT) Based NEMS Switches

To date the majority of NEMS switches have been CNT based. CNTs have been used heavily in NEMS devices because they are well characterized both chemically and physically, have low mass, exceptional directional stiffness, and good reproducibility. A number of
different CNT based NEMS switch designs have been fabricated and demonstrated over the last decade, ranging from horizontally oriented cantilevers [41, 135] and doubly-clamped devices [117, 226, 61] suspended above actuation electrodes, to vertically grown CNTs whose mechanical structures double as actuation electrodes [103, 104, 102, 101].

Some of the earliest examples of CNT based switches include CNT based nano-tweezers. The tweezers, shown in figure 2.14, consist of two parallel CNTs separated by a small gap and are drawn together by application of an electrostatic load. The devices behave just as an electrostatically actuated cantilever MEMS switch. However, instead of having a fixed electrode, both electrodes (the CNTs) are deflectable. While intended for use as a novel method for the measurement of the mass and electrical properties of nanoscopic materials, and also as a potential tool to enable 3-d AFM manipulation of samples [9, 119], the devices successfully demonstrated the use of CNTs as electrostatically actuated switches. The pull-in voltages of these devices was much lower than that of a typical MEMS switch, with Kim et al. reporting actuation of their device at $\sim 8.5$ Volts in 1999 (figure 2.14a) [119], and in 2001, Akita et al. reporting the actuation voltage for their device to be $\sim 4.5$ Volts (figure 2.14b) [9].

Since 2005 extensive work has been done by J.E. Jang et al. in the development of a low-drive voltage NEMS switch with vertically aligned CNTs. The design and operating principle behind the CNT devices developed by Jang are very similar to that of the CNT nano-tweezer devices developed previously [9, 119]. Two parallel CNTs are grown on Ni catalyst dots via a CVD bottom-up process and are designed to close upon application of an electrostatic load. While the nano-tweezers developed previously were essentially two-terminal devices, the devices developed by Jang et al. are three-terminal devices, with the third terminal acting to facilitate pull-in, or in the case of stiction, to pull the closed device apart. The original device developed in 2005 is shown in figure 2.15a and the modified device reported in 2008 is shown in figure 2.15b. The original device had a pull-in voltage of $\sim 24$ Volts [103], but the development of vertical gate terminal in the most recent devices has
allowed for pull-in voltages as low as 4.5 Volts [102]. The devices developed by Jang et al. show great potential as mechanical transistors, logic devices, non-volatile memory cells, and nano-manipulators [104, 102, 101, 107]. Similar devices for RF NEMS applications have been proposed and simulated by Dragoman et al. with results suggesting the devices would be apt for use in advanced and agile communications applications, but these devices have yet to be fabricated [59, 57].

To date, several different examples of horizontally oriented CNT based NEMS switches have been developed. These devices have out-of-plane functionality similar to most MEMS
switches and are typically fabricated using a top-down process. However, because they are CNT based, the fabrication processes must include a CNT placement step, which tends to significantly limit fabrication yield. Several examples of horizontally oriented CNT NEMS switches are shown in figures 2.16-2.19. Like the vertical CNT NEMS switch developed by Jang, and the nanotweezers developed by Kim and Akita, horizontally oriented CNT NEMS switches have a much lower pull-in voltage when compared to MEMS devices, typically between ~1.5-6 Volts.

Figure 2.16 shows an example of a three-terminal cantilever type CNT NEMS switch developed by Lee et al. in 2004. The pull-in voltage for this device was as low as 5 Volts, with $V_{GS} = 5$ Volts and $V_{DS} = 0.5$ Volts [135]. Figure 2.17 shows a novel fixed-fixed two-terminal design that employs a fabric of CNTs as the structural material. These devices developed by Ward et al. at Nantero, intended for use in non-volatile memory devices, demonstrated pull-in voltages as low as 1.4 Volts [226]. Figures 2.18 and 2.19 show fixed-fixed two-terminal CNT devices developed by Kaul et al. and Dujardin et al. The device shown in figure 2.18 had a pull-in voltage of 2.5 Volts [117], and the device shown in figure 2.19 had a pull-in voltage of 3 Volts [61].
2.2.5 Thin-film (TF) Based NEMS Switches

In the last decade, the majority of NEMS switches have been based on various CNT designs, as introduced above. In the past year however, more groups have begun to focus on top-down, TF processes, capable of more reliably producing NEMS switches [51, 54, 52, 105] having actuation voltages comparable to, or less than their CNT counterparts. The efforts put forth by [51, 54, 52, 105] have pushed the limits of top-down fabrication, producing devices with one or more dimensions < 30 nm.

In 2009 Czaplewski et al. introduced CMOS compatible TF three-terminal NEMS
Figure 2.18: A high-magnification SEM micrograph shows a single nanotube bridging a 130-nm-wide trench [117].

Figure 2.19: A two-terminal MWNT NEMS device; surface functionalized aminopropyltriethoxysilane (APTS) tracks define the preferential MWNT adsorption, allowing for MWNT placement [61].

switches with lateral functionality. They reported an actuation voltage of 13 Volts for a 5,000x100x200 nm ruthenium device, with a drain/source gap of 30 nm, and a gate-to-source gap of 50 nm, figure 2.20. Unfortunately, the fabrication process used to fabricate these devices includes many high-temperature CVD processes, resulting in an extremely low yield of only 1.5%. The low yield has been attributed to high levels of residual stress in the devices caused by the high temperature deposition of structural and masking materials [51].

In 2008 Jang et al. introduced the smallest NEMS devices ever made using traditional top-down CMOS technology, figure 2.21. Their two-terminal devices, like those reported in
Figure 2.20: SEM image of a fabricated and released laterally actuated TF NEMS switch, dimensions: 10,000 x 100 x 200 nm, with a gate gap of 70 nm and a beam gap of 50 nm [51].

[54], and in chapter 5, have embedded electrodes and out-of-plane functionality. Actuation voltages of \( \sim11 \) Volts were reported for 1,000x200x30 nm titanium nitride (TiN) cantilever devices with working gaps of \( \sim20-30 \) nm. Jang et al. used CVD TiN deposited at 250 C, thus like the devices introduced by Czaplewski et al., device performance was significantly affected by thermally induced residual stress [105].

Figure 2.21: SEM image of the smallest NEMS switch ever made using traditional CMOS technology, dimensions: 300 x 200 x 30 nm with a gap of 20 nm [105].
2.2.6  State-of-the-Art Graphene Based NEMS Switches

Since its discovery in 2005 [57] a tremendous amount of energy has gone into graphene research. Graphene has a carrier mobility of 200,000 $cm^2V^{-1}s^{-1}$ at room temperature, and a Youngs modulus of 1.5 TPa, making it the stiffest material with the highest mobility. The phenomenal material properties of graphene make it an ideal candidate for next generation electronic and NEMS devices [57, 56, 68, 72, 71].

In the past two years graphene has been implemented in NEMS for use in non-volatile memories [140, 204]. In 2008 Standley et al. developed graphene switches with nanoscale gaps created via electrical breakdown of the graphene sheets, figure 2.22. The devices are actuated electrostatically, just as the NEMS switches presented in sections 2.2.4-2.2.5, however unlike typical NEMS and MEMS electrostatically actuated switches, the devices are not electromechanically deformed. Instead, upon application of a gate bias, linear chains of carbon atoms span the break junction, thereby increasing the conductance of the device. This was verified statistically by the identification of conductance steps proportional to the conductance quantum $G = 2e^2/h$. The actuation voltage of the devices was also identified statistically, and found to be $\sim 2.8$ Volts [204].

![Figure 2.22: SEM image of the graphene NEMS device before (left panel) and after breakdown (right panel). The arrows indicate the edges of the nanoscale gap [204].](image)

Also in 2008, Li et al. reported the development of bi-stable NEMS nano-cable devices, figure 2.23. The device is composed of an amorphous $SiO_2$ wire, coated by 5-10 nm of
graphene, that spans two electrodes. The devices operate similarly to the break-junction devices developed by Standley et al., in that upon application of an applied bias between the electrodes chains of carbon span gaps created by electrical breakdown at defect sites in the graphitic layers. The actuation voltage for these devices was reported to be $\approx 4$ Volts, which, just like the devices developed by Standley, is comparable to CNT based NEMS switches. Furthermore, the devices were operated stably when irradiated by 8 keV X-rays and subjected to ambient temperatures in excess of 200 C [140, 204].

Figure 2.23: SEM image of a $G$-$SiO_2$ nanocable two-terminal device, and a high-resolution TEM image of a $G$-$SiO_2$ nanocable, showing an amorphous $SiO_2$ core, with surrounding discontinuous graphitic sheets marked with a G [140].

In 2009 Dragoman et al. proposed a graphene based RF NEMS switch, hypothesizing that the extreme stiffness and low mass of graphene could enable RF devices with opera-
tional frequencies in excess of 10 GHz. Thus far the device has been modeled and studied numerically, but not fabricated. The simulation results suggest that a graphene-based RF NEMS switch could be a significant advancement in the merger between nano-electronics and communications devices [56].

2.2.7 MEMS and NEMS Logic

The potential for mechanical computing via electromechanical systems has been recognized since the inception of MEMS switches, but while seemingly all papers regarding MEMS/NEMS switches refer to their potential applications in logic, very few have actually reported anything more than the actuation voltage of their switches. Bergstrom et al. reported to have fabricated a complete MEMS digital logic family as early as 1990. The devices were electrostatically actuated with a threshold voltage of 15 Volts and intended for use in low speed applications requiring radiation immunity. In their 1990 paper the operating principles for the entire family of microslider logic devices was proposed, but logic operation was never demonstrated [20]. Likewise, in 2000 Chae et al. proposed an electrostatically driven lateral micromechanical switch capable of inverter operation, however the group only characterized the switching behavior of their device [36].

Within the past two years however, MEMS inverters have been fabricated and demonstrated by W. Jang et al. and T Yokota et al. The devices developed by both groups are analogous in their design and operation to CMOS inverters. A diagram illustrating the analog between a MOSFET transistor and three-terminal MEMS switch, as well as a CMOS inverter and CMEMS inverter, is presented in figure 2.24. The devices developed by Jang et al. and their associated voltage transfer characteristics are shown in figures 2.25a,b. In their MEMS inverter, two three-terminal MEMS switches (MEMS transistors) are fabricated with common gate and drain terminals, but the sources are complementarily biased, thus enabling inverter operation. The fabricated MEMS switches demonstrated nearly ideal on/off characteristics, with an essentially zero off-state leakage current, a near zero sub-threshold swing
(SS < 4 mV/decade), a high on/off current ratio exceeding $10^5$, and nearly ideal transfer characteristics.

Figure 2.24: Schematic and equivalent circuit symbol of the (a) MOSFET (b) MEMS switch (c) CMOS inverter (d) CMEMS inverter [104].

The CMEMS inverter developed by Yokota et al. uses a six-terminal design and is based on the same inkjet printing fabrication technology used by Nakano [167] in the development of flexible MEMS switches. A schematic of the plastic CMEMS inverter developed by Yakota is shown in figure 2.26. While these devices operate based on the same principle as those
developed by Jang, they are novel in their design and structure. The use of flexible technology allows the device to be fabricated in a stack of bonded materials, thus requiring only one moving structure. Switching dynamics of the plastic CNEMS device were characterized and are shown in figure 2.27 [236].

2.2.8 State-of-the-Art MEMS and NEMS Logic

In the past year several papers have been published reporting the successful development of MEMS and NEMS logic devices. Spanning 2009 and 2010, two novel MEMS devices have been reported by Professor Liu’s group at Berkeley capable of the logical NOT operation, with one of the two devices also capable of a host of other logical operations [109, 168, 110]. In 2010 Professor Merhegany’s group at Case Western published a paper citing their successful development of a complementary NEMS silicon carbide (SiC) based inverter operated at temperatures as high as 500° C [136]. These devices represent the current state of the art in MEMS and NEMS logic devices as well as electromechanically actuated switches.
Figure 2.26: a) A plastic CMEMS device with six terminals (right) and a plastic MEMS switch with four terminals (left). In both switches, the cantilever beam is pulled, and brought in contact with the switch sheets via an electrostatic attraction; b) A cross-sectional illustration of the plastic CMEMS inverter. All of the electrodes are fabricated via ink-jet printing [236].

Figure 2.27: Dynamic operation/ characterization of the plastic CMEMS inverter [236].
2.2.8.1 MEMS: 4-terminal Relay

A 4-terminal MEMS relay technology for complementary logic was introduced by Professor Liu’s group in 2009. The design is novel in that it includes body electrodes that allow the actuation voltage of the device to be electrostatically tuned. The addition of the fourth body electrode not only allows the device’s actuation voltage to be tuned but also allows the relay to mimic the operation of either p or n-channel MOSFETS [168]. The devices reported exhibited low switching voltages, < 2 V, low mechanical delay, < 100 ns, and demonstrated lifetimes greater than 1 billion cycles.

A schematic of the device developed by Nathanael et al. is shown below in figure 2.28. The fabrication process is CMOS compatible. All electrodes are DC sputtered tungsten, and the structural material is boron-doped LPCVD poly-silicon deposited at 410 C, and for wear protection a thin layer of ALD titanium oxide was grown on the device following release.

![Figure 2.28: SEM image of the 4-terminal relay developed by Professor Liu’s group at Berkeley. The suspended plate has an approximate area of 27 x 27 \( \mu m^2 \), [168].](image)

The waveform for the 4-terminal relay is shown in figure 2.29. The voltage applied to
the body electrodes was adjusted to 10.6 V and 8.9 V to achieve symmetric switching at low voltage. The device was operated at 50 Hz with $V_{DD} = 2$ V and $V_{ss} = 0$ V.

![Figure 2.29](image)

The primary setback for this device is that it is not a true complementary inverter. While the device has been tuned to display symmetric switching at low voltages allowing for complementary like inverter operation, this can only be achieved by applying voltages of $\approx \pm 10$ V to the body electrodes. Thus, while the apparent operational voltage $V_{DD} = 2$ V is compatible with existing silicon technologies, the device would require a secondary voltage source for biasing of the body electrodes – one that is not CMOS compatible.

### 2.2.8.2 MEMS: Seesaw Relay

Using the same fabrication technology as for the 4-terminal relay design Liu et al. also developed a perfectly complementary seesaw relay device [109, 110]. The device which is an electrostatically actuated torsional switch resembling a seesaw, hence the name, is shown in figure 2.30. The seesaw design uses a single moveable plate (the gate electrode) anchored by two torsion beams that allow the free ends of the plate to be displaced up and down in a perfectly complementary fashion. The device is controlled by two body electrodes that are located on either side of the torsional axis, which are used to pull the torsional switch.
(gate) into contact with either a left or right pair of coplanar source and drain electrodes. The arms on either side of the gate are electrically isolated from the gate, and upon contact bridge the biased source and drain electrodes.

Figure 2.30: schematic: (a) CAD model of the seesaw relay, and definitions of design parameters. In this work, $T_{\text{GAP}} = 0.2 \, \text{um}$, $T_{\text{CONTACT}} = 0.1 \, \text{um}$, $L = 3 \, \text{um}$, $W = H = 1 \, \text{um}$, $L_C = 7.5 \, \text{um}$, $W_C = 2 \, \text{um}$, $L_A = 42 \, \text{um}$, $L_{A1} = 12 \, \text{um}$, and $W_A = 40 \, \text{um}$. (b) Schematic cross-sectional views from (a). OFFON and ONOFF (shown here) are the two stable states for perfectly complementary operation [109, 110].

The seesaw design has been successfully used to demonstrate several different logic functions such as buffer, NOT, AND and OR. Waveforms for these functions are shown in figure 2.31. The devices have also been configured to form a bistable latch. By adding a transistor the group successfully constructed an SRAM cell. All of these functions can be implemented using a single seesaw relay with drain electrodes connected to form an output node and appropriate bias conditions [109, 110]. For these operations the gate to body bias ($V_{GB}$) used to actuate the device was $\approx 7 - 10 \, \text{V}$. To avoid micro-welding issues $V_{DS}$ was limited to 2 Volts.

Just as with the 4-terminal relay, the see-saw relay is CMOS compatible in a materials and fabrication technology sense, but incompatible in an operational voltage sense. However,
because of its symmetric design, the see-saw design is essentially two devices in one (a left and right device) [110], which increases the functional density of the device. With further scaling as nano-fabrication techniques become more advanced, and with improved design optimization, the devices will have a superior advantage over other CMOS compatible MEMS or NEMS logic devices having only one operation per device. Therefore, this seesaw architecture has a tremendous advantage over typical MEMS or NEMS logic architectures which are typically based on constructing logic devices from fundamental building blocks – usually 3-terminal switches. The versatility of this design is unmatched and truly state-of-the-art.

2.2.8.3 NEMS: High Temperature Computing

Replacing existing complementary metal-oxide semiconductor field-effect transistors with silicon carbide (SiC) NEMS switches is a promising approach for low-power, high-performance logic operation at temperatures greater than 300° C, beyond the capability of conventional silicon technology [136]. Professor Mehregany’s group at Case Western has developed 3-terminal switches capable of nearly zero off-state current, microwave operating frequencies, and radiation hardness, at nanoscale dimensions.

The device reported is a micro-machined NEMS SiC inverter operated at temperatures greater than 500° C with ultra-low leakage current. The inverter is composed of two laterally actuated NEMS cantilever switches following a complementary static-CMOS logic style that consists of pull-up and pull-down stages. Each switch is 3-terminal having a source, gate and drain. This logic style was chosen because it provides low noise sensitivity and low static-power consumption [136].

The cantilevers (sources) used to construct the inverter are both 8 um long, 200 nm wide, and 400 nm thick. The source to gate gap height is \( \approx 150 \) nm. The SiC is a heavily nitrogen-doped polycrystalline 3C-SiC film deposited by low-pressure chemical-vapor deposition. All geometric features are patterned via e-beam, and the SiC is etched via DRIE in
a $SF_6$ environment. The SiC device is shown below in figure 2.32.

The inverters were operated at 500 kHz with $V_{DD} = 6$ V and $V_{SS} = -6$ V, which is higher than Si logic devices that typically operate at 3 V or lower. Figure 2.33 shows a waveform for the SiC inverter described. Furthermore, the devices characterized by Professor Mehregany’s group proved to have stellar reliability. Device lifetimes were reported in excess of 21 billion cycles at 25° C and 2 billion cycles at 500° C. While these devices currently have actuation voltages incompatible with state-of-the-art CMOS technologies, they are clearly a huge technological advancement for high temperature logic devices and represent the current state-of-the-art in NEMS logic devices.

The scaling down of CMEMS inverters to CNEMS inverters should allow for devices with operational voltages comparable to and compatible with CMOS technologies; however, to date very few CNEMS logic devices have been reported. The devices described above are the the most recent devices reported, and as stated represent the current state-of-the-art in the field. Until very recently the focus seems to have been on the next generation of electrical devices, called non-CMOS nanoelectrical devices. These devices include CNT FETs and nanowire (NW) FETs [84]. As an analog to MOSFETS, CNTs and NWs used in the nanodevice serve the same function as the doped channel in the bulk substrate of a CMOS device. The use of CNTs or NWs in place of a doped conducting channel is preferable because electrical transport in these materials is typically ballistic at room temperature [58, 84, 106, 152]. To date Bachtold et al. have demonstrated an AC ring oscillator, SRAM cell, inverter, NOR, and AND gates using CNT FETs; and Javey et al. have demonstrated complementary ring oscillators, NOR, OR, NAND, and AND gates based on arrays of p and n-type CNT FETS [12, 84].

** An extended literature review covering CMOS scaling, irradiation of CMOS, as well as thin-film processing techniques can be found in Appendix B.
Figure 2.31: Circuit diagram and several different waveforms for different logic operations performed by the seesaw relay developed by Liu et al. at Berkeley [109, 110].
Figure 2.32: SEM image of the SiC NEMS inverter developed at Case Western [136]

Figure 2.33: Waveform of a SiC NEMS inverter developed at Case Western. This devices was operated at 500 kHz with $V_{DD} = 6$ V and $V_{SS} = -6$ V [136]
3.1 Overview

In all engineering disciplines sufficient mathematical models are of the utmost importance. By sufficient it is meant a model that can accurately approximate the behavior of a system, whether that system be mechanical, electrical, or chemical to a degree of exactness deemed acceptable by the engineer. Models may be used to aid in the design of a system, leading to more intelligent and optimal designs, while minimizing time and money spent on the physical design/fabrication process. Models are also used to study the physics of a given system in detail through numerical experiments. Numerical experiments can elucidate design rules or system responses that may have been difficult to identify through the physical design or experimental process. A good model can be the most important tool an engineer or scientist has.

In this chapter analytic modeling applicable to the design and study of thin-film NEMS switches is described in detail. These models approximate the pull-in voltage of devices having symmetric, non-rectangular profiles, as well as a variety of physically significant phenomena specific to devices with gap heights in the nano-regime (typically < 100 nm). These phenomena include the non-linear effect of the van der Waals force on the static and dynamic behavior of MEMS/NEMS devices and the pre-actuation tunneling current that is often measured experimentally [129, 48, 85]. The aim of the chapter is to give a set of
analytic formulations that may aid in the design and understanding of more complicated MEMS/NEMS structures. It is my hope that these models may be of use in particular to the engineer who does not have access to more sophisticated computer software.

3.2 Effective Stiffness of Two or Three Terminal MEMS/NEMS Switches having Symmetric Non-Rectangular Profiles

In the following section expressions for the effective stiffness of beams with rectangular and symmetric non-rectangular profiles subjected to fully and partially distributed loads are derived. The derivations are shown in detail to provide a firm understanding of the derivation process, underlying equations, and methods. In this way, if one wished to derive the effective stiffness for even more complicated geometries, one would simply need to follow the framework presented here. The derivation of effective stiffness will allow the calculation of the pull-in voltage of electrostatically actuated two or three-terminal MEMS and NEMS devices, and in fact, the analysis could be extended for n-terminal scenarios.

3.2.1 Rectangular Profiles

We will derive the pull-in voltages for 2 or 3 Terminal MEMS/NEMS switches that have Symmetric-Non-Rectangular profiles using energy methods and plane strain assumptions. Profiles considered are the Bow-tie, which is a prevalent design for MEMS RF switches, and profiles constructed by \( n^{th} \) order polynomials which have been dubbed "Poly-tie". Examples of the different profiles are shown below in figures 3.1 and 3.2.

Energy methods offer a simple and elegant solution for the derivation of the effective stiffness of a beam subjected to a particular load. For this derivation Castigliano’s second theorem [17], equation 3.1, will be used to derive an expression for the displacement of a fixed-fixed beam of constant width subjected to a point load at some distance \( a \) from a fixed end, figure 3.4. The displacement will then be used to calculate the effective stiffness of the beam.
Figure 3.1: Schematic of the Bow-tie structure as seen in the x-z plane. $W_M$ is the maximum half-width, $W_o$ the minimum half-width, and $L$ the length.

Figure 3.2: Schematic a general poly-tie structure as seen in the x-z plane. $P(x)$ is an $n^{th}$ order polynomial that fits some profile, $W_M$ is the maximum half-width, $W_o$ the minimum half-width, and $L$ the length.
\[ u_i = \frac{\partial U}{\partial F_i} \]
\[ \theta_i = \frac{\partial U}{\partial M_i} \]  

(3.1)

We first derive an expression for the strain energy of a deformed beam. This can be accomplished by considering a general stress-strain curve for some material (the curve shown here is for a general metal), figure 3.3. The shaded area beneath the curve is the strain energy per unit volume in the elastic regime. We only consider the energy stored in the system in the elastic regime because any further stressing of the beam beyond the yield stress results in permanent deformation of the beam, and thus dissipation some of the stored energy. Thus we only consider the conservative energy regime.

The strain energy per unit volume is thus given by,

\[ u_{vol} = \frac{1}{2} \sigma \epsilon \]  

(3.2)

Thus the total strain energy in the beam is found by integrating, \( u_{vol} \), over the volume of the beam.

\[ U = \frac{1}{2} \int_V \sigma \epsilon dV \]  

(3.3)

The internal stress of a beam subjected to a bending moment is given by,

\[ \sigma = \frac{M}{I} y \]  

(3.4)

where \( I \) is the bending moment of inertia and is defined in figure 3.4. Thus using equation 3.4 with 3.5 we have the total strain energy of a deformed beam as a function of the applied bending moment \( M \).

\[ U = \frac{1}{2EI} \int_V M(x)^2 dV \]  

(3.5)

Thus, to calculate the stain energy of a deformed beam we must know the applied moment \( M \) as a function of the beam’s length. This is accomplished via Newton’s 3rd law.
Figure 3.3: General $\sigma - \epsilon$ curve for metal. The strain energy for a material stressed in the elastic-regime is shaded.
The free-body diagram for a fixed-fixed beam subjected to a load $F$, at some distance $a$ from a fixed end is given in figure 3.4.

The sum of forces in the y-direction gives,

$$\sum F_y = 0 = R_A + R_B - F \implies F = R_A + R_B (3.6)$$

and the sum of moments about point $A$ gives,

$$\sum M = 0 = -M_A + M_B - Fa + R_B L \implies M_B = M_A + Fa - R_B L \quad (3.7)$$

To calculate $M(x)$ we apply Newton’s 3rd law to the two sections of the beam.

### 3.2.2 Section 1: $0 \leq x < a$

$$\sum F_y = 0 = R_A + V(x) \implies R_A = -V(x) \quad (3.8)$$

$$\sum M = 0 = -M_A + M_1(x) + V(x)x \implies m_1(x) = M_A + R_A x \quad (3.9)$$

### 3.2.3 Section 2: $a < x \leq L$

$$\sum F_y = 0 = R_B + V(x) \implies R_B = -V(x) \quad (3.10)$$

$$\sum M = 0 = M_B - M_2(x) - V(x)(L - x) \implies M_2(x) = M_B + R_B(L - x) \quad (3.11)$$

Now using equations 3.9 and 3.11, equation 3.5 becomes,

$$U = \frac{1}{2EI} \left( \int_0^a M_1(x)^2 dx + \int_a^L M_2(x)^2 dx \right) \quad (3.12)$$

Evaluating equation 3.13 we have,

$$U = \frac{1}{2EI} \left( M_A^2 a + M_A R_A a^2 + \frac{R_A^2}{3} a^3 + \frac{(M_B + (1-a)R_B)^3 - M_B^3}{3R_B} \right) \quad (3.13)$$
Figure 3.4: A fixed-fixed beam subjected to a point load acting at some distance $a$ from the left support, and the associated free-body diagram.

Figure 3.5: Free-body diagram for $0 \leq x < a$ of a fixed-fixed beam subjected to a point load acting at some distance $a$ from the left support.

Figure 3.6: Free-body diagram for $a < x \leq L$ of a fixed-fixed beam subjected to a point load acting at some distance $a$ from the left support.
By applying Castigliano’s 2nd theorem to the boundary conditions of the structure we can solve for all of the currently unknown reaction forces. Applying Castigliano’s theorem to the left boundary we have,

\[
\frac{\partial U}{\partial M_A} = \theta_A \\
\frac{\partial U}{\partial R_A} = u_A
\]  

(3.14)

where the boundary conditions here are \( \theta_A = u_A = 0 \). Thus we can set equations 3.14 equal to each other and solve for the unknown \( M_A \). We next use equations 3.8 and 3.9 with equation 3.14 to solve for the unknowns \( R_B, M_B, \) and \( R_A \). The derived reaction forces are:

\[
M_A = -\frac{Fa(L-a)^2}{L^2} \\
M_B = \frac{Fa^2(a-L)}{L^2} \\
R_A = \frac{F(L-a)^2(L+2a)}{L^3} \\
R_B = \frac{Fa^2(3L-2a)}{L^3}
\]  

(3.15)

Now that all of the reaction forces are known we need to calculate the displacement as a function of \( x \) along the length of the beam. This is done by solving the second order ODE, equations 3.16, that describes the system subject to the boundary conditions for a fixed-fixed beam, \( y(0) = y'(0) = 0 \), [17]. For \( 0 < a \) we have,

\[
EIy''(x) = -M_1(x) = -M_A - R_A(x) \\
EIy'(x) = -\frac{R_A}{2}x^2 - M_Ax + C \\
EIy(x) = -\frac{R_A}{6}x^3 - \frac{M_A}{2}x^2 + Cx + D
\]  

(3.16)

Via application of the boundary conditions the displacement for a concentrated load \( F \) is found to be,

\[
y(x) = -\frac{1}{EI} \left( \frac{R_A}{6}x^3 + \frac{M_A}{2}x^2 \right)
\]  

(3.17)

At this point in the derivation we have successfully calculated the displacement of a fixed-fixed beam with constant width subject to a concentrated load \( F \). However, the MEMS
and NEMS devices studied in this thesis are subject to loads distributed over some region of their length. Fortunately, the previous derivation was not done in vain because using linear superposition we can easily calculate the displacement of a fixed-fixed beam subject to a distributed load [186].

First we define the distributed load over the entire length of the beam to be,

\[ \xi = \frac{F}{L} \quad (3.18) \]

Thus using equations 3.18 and 3.15 with equation 3.17 we have,

\[ y(x, a) = \frac{1}{6EI L^3} (\xi x^2(a - L)^2(3aL - 2ax - Lx)) \quad (3.19) \]

Where the displacement is now written as a function of \( x \) and \( a \). The fixed-fixed devices studied in this thesis are designed such that the maximum deflection occurs at center of suspended structure. The deflection at the center of the beam resulting from the application of some distributed load, shown in figure 3.7, can be calculated by evaluating equation 3.19 at \( x = L/2 \) and summing the contributions from point loads over the region that they are distributed, equation 3.20. In general, the displacement at any point \( x \) due to any distributed load can be calculated using equation 3.20 by simply evaluating 3.19 at that point.

\[ u = \int_{c}^{b} y(L/2, a) da \quad (3.20) \]

3.2.4 Fixed-fixed Beam Subjected to a Fully-Distributed Load

As a check of the preceding derivation, we consider the maximum displacement of a fixed-fixed beam subjected to a fully-distributed load, shown in figure 3.8. The displacement is calculated by evaluating 3.19 at \( x = L/2 \), and because of symmetry, integral 3.20 is multiplied by 2 and evaluated from \( L/2 \rightarrow L \), equation 3.21.

\[ u = 2 \int_{L/2}^{L} y(L/2, a) da \quad (3.21) \]
Figure 3.7: Fixed-fixed beam subjected to a distributed load $\xi$

Figure 3.8: Fixed-fixed beam subjected to a fully-distributed load $F/L$
Evaluating equation 3.21 at $L/2$ and integrating over the length of the beam the displacement is calculated to be,

$$u = \frac{\xi L^4}{384EI} \implies u = \frac{FL^3}{384EI}$$

which is exactly the formula given by [17, 186] for the maximum displacement of a fixed-fixed beam subject to a fully-distributed load, figure 3.8.

Because the derivation of displacement for a given load considered only the linear regime of the stress-strain curve, it was implicitly assumed that displacements are small, therefore the relationship between applied load and displacement can be approximated by Hooke’s law: $K_s u = F$. Using the above example, the spring constant of the system is given by,

$$K_s = \frac{384EI}{L^3}$$

For thin-film devices the effective stiffness of a system also includes a contribution from the tensile stress in the film. For the sake of brevity, and because residual stress is not studied in this thesis, this contribution will not be discussed in detail here. More information regarding residual stress can be found in [186]. From [186] the stiffness contribution from thin-film stress is given by,

$$K_\sigma = \frac{8\sigma_x(1-\nu)wt}{L}$$

where $w$ and $t$ are the width and thickness of the considered device.

Finally, the effective stiffness of a fixed-fixed device with constant width is the sum of the contributions from geometry and stress, and is thus given by equation 3.25.

$$K_{eff} = \frac{384EI}{L^3} + \frac{8\sigma_x(1-\nu)wt}{L}$$

Up to this point the derivation presented has been specifically for beams of constant width, which implies constant moment inertia. Although the equations derived are well
documented in the literature, the derivation has been presented in detail here so that we may have a fundamental understanding of the problem starting from a static analysis of the forces on the system. This way we have derived the proper equations to extend the derivation to include structures whose widths vary with length. It is important to note that the geometries considered here, Bow-tie and Poly-tie, are symmetric across the x-y plane, figures 5.27 and 3.2. This condition allows us to continue to use plane strain assumptions and a 2-D model. The application of a distributed load to an anti-symmetric structure would induce unbalanced moments, with respect to the x-y plane, that would lead to a twisting mode of deformation that cannot be captured by a 2-D model. Thus, if one were to consider an anti-symmetric profile then a significantly more complicated 3-D model would be needed.

3.2.5 Non-rectangular Profiles

The first symmetric and non-rectangular structure that we will consider is the Bow-tie structure whose profile is illustrated in figure 5.27, along with the key geometric parameters: \( W_M \) and \( W_o \). \( W_M \) is the maximum half-width of the structure, while \( W_o \) is the minimum half width of the structure. Because these structures are of varying width, the first step of the derivation is to derive the half-width function. The beam symmetry across the y-z plane implies that we only need to consider the half-width function for \( 0 \leq x' \leq \alpha/2 \), or \( \alpha/2 \leq x' \leq L \), as was stated in equation 3.21.

The structure’s half-width function is given by the following piece-wise function,

\[
\begin{align*}
  z(x') &= \begin{cases} \\
  W_o & \text{for } 0 \leq x' \leq \alpha/2 \\
  2 \left( \frac{W_M - W_o}{L - \alpha} \right) x' + \frac{W_o L - W_M \alpha}{L - \alpha} & \text{for } \alpha/2 < x' \leq L \\
  \end{cases} \\
  \text{where, } x' &= x - L/2 ;
\end{align*}
\]

(3.26)
The width function is thus,

\[ w(x) = 2z(x); \] (3.27)

Now, the bending moment of inertia \( I \) is a measure of a beam’s resistance to bending moments at a particular location along it’s length. Therefore, for a load applied at some distance \( a \), as seen in figure 3.4, the bending moment of inertia for a structure whose width varies with length will be given by equation 3.31.

\[ I(a) = \frac{1}{6}z(a)t^3; \] (3.28)

We can now use the equations for the structure’s width and bending moment of inertia, 3.31 and 3.27, with the previously derived equation for the mid-point displacement of a fixed-fixed beam subject to a distributed load, equation 3.21, to derive the analytic equation for the mid-point displacement of a fixed-fixed Bow-tie structure subject to a fully-distributed load, equation 3.29.

\[
\begin{align*}
\frac{1}{4E} &= -\frac{1}{24E} \left[ \int_{L/2}^{(L+\alpha)/2} \frac{(L-a^2)(L-4a)}{I_1(a-L/2)} da + \int_{(L+\alpha)/2}^{L} \frac{(L-a^2)(L-4a)}{I_2(a-L/2)} da + \int_{L}^{L} \frac{(L-a^2)(L-4a)}{I_3(a-L/2)} da \right] \\
\Rightarrow & -\frac{1}{4E} \left[ \int_{L/2}^{(L+\alpha)/2} \frac{(L-a^2)(L-4a)}{W_o} da + \int_{(L+\alpha)/2}^{L} \frac{(L-a^2)(L-4a)}{2(W_o-W_M)(a-L/2)+(W_M \alpha-W_o L)} da \right] 
\end{align*}
\] (3.29)

The same methodology is applied to derive the mid-point displacement of a fixed-fixed Poly-tie structure subjected to a distributed load. First a half-width function fit by some \( n^{th} \)-polynomial is constructed, which we will call \( P(x) \). This implies that the width and bending moment of inertia for a poly-tie structure is given by,

\[ w(x) = 2P(x); \] (3.30)

\[ I(a) = \frac{1}{6}P(a)t^3; \] (3.31)
Thus using equation 3.21, the mid-point displacement of a fixed-fixed Poly-tie structure subject to a distributed load over its entire length is given by,

\[ u_{PT} = -\frac{1}{4Et^3} \left[ \int_{L/2}^{L} \frac{(L - a^2)(L - 4a)\xi}{P(a)} da \right] \]  

(3.32)

Once the mid-point displacement for either profile has been calculated, the stiffness \( K_s \) may be extracted via substitution of equation 3.18 and Hooke’s law, as was done in equation 3.22 for a beam of constant width. Using the derived width functions for Bow/Poly-tie structures it follows that the contribution to the stiffness resulting from thin-film tensile stress is simply,

\[ K_\sigma = 2 \left( \int_{L/2}^{L} \frac{8\sigma_x(1 - \nu)W(x)t}{L} dx \right) \]  

(3.33)

### 3.2.6 Partially Distributed Loads

So far the analysis presented has considered beams subjected to fully-distributed loads. As will be seen in chapter 5, several different switches have been fabricated and characterized as part of this thesis effort, including 2-terminal WALD NEMS switches, for which the preceding analysis specific to a fully-distributed load is perfectly valid. However, for 3-terminal WALD NEMS switches, and even some types of 2-terminal switches (depending on the electrode lay-out/fabrication process) developed by this work, a fully-distributed model does not represent electrostatic loading of these devices. These devices are more accurately modeled by partially distributed loads. Fortunately, using the framework developed in this section the analytic derivation of \( K_s \) for partially distributed loads is rather straightforward.

There are two loading cases that are particularly relevant to the devices studied during the course of this research. The first case is that of a load distributed symmetrically about the beam’s mid-point (centrally-distributed load), figure 3.9. This loading case is an appropriate representation of a 2-terminal switch whose gate electrode is centered beneath the suspended
beam/source, but whose width is some percentage of the overall beam length, fig 3.10; or a drain-to-source biased 3-terminal switch, as developed in chapter 4, whose drain terminal is centered beneath the the source, figure 3.11. The second loading case, called here a bi-distributed load, figure 3.12, is representative of a gate-to-source biased 3-terminal switch, whose gate-electrode geometry is configured as shown in figure 3.13.

For partially distributed loads, derivation of effective stiffness is identical except for one small detail. The relationship of force to unit length is no longer simply some load $F$ divided the length of the beam, as given previously in equation 3.18. For the two loading cases described the relationship between the point load $F$ and the distributed load, $\xi$ is now given by the following equations [186],

$$\xi = \frac{F}{2(x - L/2)}, \text{ loading case 1} \tag{3.34}$$

$$\xi = \frac{F}{2(L - x)}, \text{ loading case 2} \tag{3.35}$$

Thus the general equations for the mid-point displacement of a fixed-fixed beam, having a symmetric profile, and subject to the partially distributed loads described are given by,

$$u = -\frac{1}{24E} \left[ \int_{L/2}^{x} \frac{(L - a^2)(L - 4a)\xi}{I(a)} \, da \right], \text{ loading case 1} \tag{3.36}$$

$$u = -\frac{1}{24E} \left[ \int_{x}^{L} \frac{(L - a^2)(L - 4a)\xi}{I(a)} \, da \right], \text{ loading case 2} \tag{3.37}$$

Again, once the mid-point displacement for either profile has been calculated the stiffness $K_s$ may be extracted via substitution of equation 3.34/3.35 and Hooke’s law.

### 3.3 Pull-in of 2 or 3 Terminal Bow/Poly-tie MEMS/NEMS Switches

The analytic derivation of displacement versus applied voltage for a 1-D lumped mass is no different for Bow/Poly-tie MEMS/NEMS devices than it is for typical reported devices
Figure 3.9: Fixed-fixed beam subjected to a centrally-distributed load

Figure 3.10: A 2-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source; a distributed load similar to that shown in figure 3.9 represents the electrostatic load applied to this device

Figure 3.11: A 2-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source biased by $V_{DS}$; a distributed load similar to that shown in figure 3.9 represents the electrostatic load applied to this device
Figure 3.12: Fixed-fixed beam subjected to a bi-distributed load

Figure 3.13: A 3-terminal MEMS/NEMS switch with drain electrode centered beneath suspended source, and geometrically symmetric, electrically connected gate electrodes biased by $V_{GS}$; a distributed load similar to that shown in figure 3.12 represents the electrostatic load applied to this device
having rectangular profiles. The derivation is well documented, and was reported as early as the mid 1960’s by Nathanson [171]. Therefore a derivation of the expression for voltage as a function of device displacement is omitted, and the expression is given without further explanation, equation 3.38.

It should be noted that more accurate, and complicated 2-D distributed load models have been derived and reported, but these are beyond the scope of analytic work in this dissertation. The primary difference between the models is that distributed load models predict pull-in to occur at displacements corresponding to $\approx 40 - 50\%$ of the initial gap height 3.38, and 1-D lumped mass models predict a more conservative pull-in height of $\sim 1/3$ the initial gap height.

\[ V(y) = \sqrt{\frac{2K_{eff}y(g_o - y)^2}{\epsilon_o A}} \]  

(3.38)

Where: $y$ is the displacement, $K_{eff}$ the effecting stiffness of the suspended structure, $g_o$ the initial gap height, $\epsilon_o$ the permittivity of free space, and $A$ the structural area that the distributed load is applied over.

3.3.1 Analytic Case Studies: Displacement Vs. Applied Voltage for Rectangular, Bow-tie, and 2nd Order Poly-tie WALD NEMS 2 and 3-terminal Switches

Using the theory derived in this section plots of displacement versus applied voltage have been generated for fixed-fixed rectangular, bow-tie, and poly-tie switches subject to the three loading cases described (fully-distributed, centrally distributed, and symmetrically centered near the anchors). The loading cases correspond to the electrostatic loading of a 2-terminal switch with a gate/source overlap area = 100%, a 3-terminal switch actuated by the drain electrode, and a 3-terminal switch actuated by the gate electrode.

All of the devices modeled have similar dimensions so that their respective switching
behaviors can be compared. The devices modeled here have been designed to represent feasible designs for WALD NEMS 2 and 3 terminal switches. Thus all material properties correspond to that of bulk W, and all dimensions are representative of actual device that can be fabricated using the fabrication processes developed by this research effort, presented in chapter 5.

For these case studies each device has the following dimensions in common: \(L = 5\) um, \(W_o = 250\) nm, \(t = 32\) nm, \(D_W = \frac{L}{4}\), \(g_{DS} = 20\) nm, and \(g_{GS} = 50\) nm. For the bow-tie and poly-tie profiles \(W_M = 3.5\) um. A schematic detailing device geometries visible in a cross-section defined by the x-y plane is given by figure 3.14, and the other parameters \(W_o\) and \(W_M\) for bow-tie and poly-tie devices have previously been defined in figures 3.1 and 3.2.

### 3.3.1.1 Displacement Vs. Applied Voltage for 2 and 3-terminal Switching

In figures 3.15-3.17 displacement versus applied voltage has been plotted for each device subject to the different loading cases described. For the dimensions chosen we see that the pull-in voltage for gate actuation is much larger than for either of the other two loading cases for all of the modeled devices. This is to be expected when comparing the gate actuated devices to the 2-terminal devices, because for these cases the gap-heights are the same, whereas for the gate actuated case the total overlap area is less, and from equation 5.3 we see that the pull-in voltage is inversely proportional to \(A^{1/2}\).

Although the \(A_{DS}\) is smaller than \(A_{GS}\) for the other loading cases, \(g_{DS}\) is more than 50% less than \(g_{GS}\). From equation 3.38 we see that the pull-in voltage is directly proportional to \(g_{DS}\), thus for the ratio of dimensions chosen \(V_{\text{pullin,DS}}\) is less than both \(V_{\text{pullin,GS}}\) and \(V_{\text{pullin,2T}}\) for all of the devices investigated. In chapter 5 it will be shown that device geometries can be constructed such that \(V_{\text{pullin,GS}} > V_{\text{pullin,DS}}\).
Figure 3.14: 3-terminal Device schematic (x-y plane); here: L := device length, $D_W$ := drain width, $G_W$ := gate width, $g_{GS}$ := source-to-gate gap height, and $g_{DS}$ := source-to-drain gap height.

Figure 3.15: Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices (rectangular profile); Dimensions: 5,000 x 500 x 32 nm (S); $D_W = 1.250 \text{ um}$, $g_{GS} = 50 \text{ nm}$, $g_{DS} = 20 nm$, and for a fully-distributed load (2-terminal switching) $g_{GS} = 50 \text{ nm}$.
Figure 3.16: Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices (bow-tie profile); Dimensions: $L = 5 \ \mu m$, $W_o = 250 \ \text{nm}$, $W_M = 3.5 \ \mu m$ (S); $D_W = 1.250 \ \mu m$, $g_{GS} = 50 \ \text{nm}$, $g_{DS} = 20\text{nm}$, and for a fully-distributed load (2-terminal switching) $g_{GS} = 50 \ \text{nm}$

Figure 3.17: Displacement Vs. Applied Voltage for 2 and 3 terminal WALD NEMS devices ($2^{nd}$ order poly-tie profile); Dimensions: $L = 5 \ \mu m$, $W_o = 250 \ \text{nm}$, $W_M = 3.5 \ \mu m$ (S); $D_W = 1.250 \ \mu m$, $g_{GS} = 50 \ \text{nm}$, $g_{DS} = 20\text{nm}$, and for a fully-distributed load (2-terminal switching) $g_{GS} = 50 \ \text{nm}$
3.3.1.2 Comparison of Displacement Vs. Applied Voltage of Each Profile

Here the curves plotted in figures 3.15-3.17 have been replotted so that each profile is directly compared for the 3 loading cases, figures 3.18-3.20. These plots make it clear that for similarly dimensioned geometries, for either 2 terminal, or gate actuated 3-terminal devices, the bow-tie and 2nd order poly-tie switches have smaller actuation voltages than rectangular switches. This is obviously because of their much higher gate-to-source over lap areas. In figures 3.18 and 3.20 the bow-tie switches have a slightly lower pull-in voltage compared to the 2nd order poly-tie switches for these loading cases. This is because $A_{GS,\text{bow-tie}}$ is approximately 10.2% and 12.2% larger than $A_{GS,\text{poly-tie}}$ for the 2-terminal and gate actuated 3-terminal cases respectively.

For the drain actuated case, figure 3.19, we see that the bow-tie and rectangular switches have the same pull-in voltage. This is because for this case the two devices have the same actuation areas, source-to-drain gap heights, and bending moment of inertias, and therefore same stiffness and switching response. Thus, it is demonstrated that a 3-terminal bow-tie switch whose rectangular span overlaps an actuating electrode behaves identically to a rectangular device of identical width. This will be further explored in the development of WALD CNEMS inverters, chapter 5. Finally figure 3.19 shows that the pull-in voltage of the 2nd order poly-tie switch is less than that of the other two cases. This is because $A_{DS,\text{poly-tie}}$ is approximately 27.1% larger than $A_{DS,\text{bow-tie}}$ or $A_{DS,\text{rect}}$.

The pull-in voltages for the cases described are concisely summarized in table 3.1.

Table 3.1: Analytic Pull-in Voltages for Rectangular, Bow-tie, and 2nd Order 2 and 3-terminal WALD NEMS switches

<table>
<thead>
<tr>
<th>Device Profile</th>
<th>$V_{\text{pullin},2T}$</th>
<th>$V_{\text{pullin},DS}$</th>
<th>$V_{\text{pullin},GS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangular</td>
<td>1.6759 V</td>
<td>0.6167 V</td>
<td>2.3078 V</td>
</tr>
<tr>
<td>Bow-tie</td>
<td>0.8660 V</td>
<td>0.6167 V</td>
<td>1.5002 V</td>
</tr>
<tr>
<td>2nd Order Poly-tie</td>
<td>1.0428 V</td>
<td>0.6519 V</td>
<td>1.665 V</td>
</tr>
</tbody>
</table>
Figure 3.18: Comparison of Displacement Vs. Applied Voltage for 2-terminal WALD NEMS devices

Figure 3.19: Comparison of Displacement Vs. Applied Voltage for 3-terminal drain actuated WALD NEMS devices
Figure 3.20: Comparison of Displacement Vs. Applied Voltage for 3-terminal gate actuated WALD NEMS devices
3.4 Non-linear Dynamics of Electromechanical System Including van der Waals Force

In the following section the effect of the van der Waals force on the non-linear system dynamics of NEMS switches is studied in detail. The static system is first studied and bifurcation diagrams generated. From these diagrams we find that depending on two system parameters, \( \alpha \) and \( \beta \), which are dependent on the Hamaker constant and applied potential, the system has either zero or two stability points. A stability analysis is then conducted to study the nature of the stability points, and phase diagrams of the system for varying system parameter plotted. Finally, expressions for the detachment lengths of a cantilever and fixed-fixed switch are derived and detachment curves plotted.

3.4.1 Equations of Motion

For this analysis the NEMS switch will be modeled by a simple 1-D mass spring system with applied electrostatic and van der Waals loads. Figure 3.21 shows the system model with applied loads and the associated free-body diagram. Now, via Newton’s second law the sum of the applied forces are set equal to the inertial force, equation 3.39. Expressions for each of the the applied loads are given by equation set 3.40. In equation set 3.40 \( k_{eff} \) is the effective spring constant of the mechanical structure considered, \( \epsilon_o \) the permittivity of free space, \( g_o \) the initial gap height between electrodes, \( y \) the current displacement, \( V \) the applied potential, and \( A_{132} \) the Hamaker constant for the system of materials, which can be calculated using the equations derived in Appendix C.

\[
F_{inex} = F_k - F_{elect} - F_{vdw}
\] (3.39)
where,

\[ F_{\text{iner}} = m \frac{d^2 y}{dt^2} \]

\[ F_k = k_{\text{eff}} (g_o - y) \] \hspace{1cm} (3.40)

\[ F_{\text{elect}} = \epsilon_o \frac{Lw}{2y^2} V^2 \] \hspace{1cm} (3.41)

\[ F_{\text{vdw}} = \frac{A_{132} Lw}{6\pi y^3} \] \hspace{1cm} (3.42)

Thus the equation of motion for a MEMS or NEMS device including the influence of van der Waals force, is given by,

\[ m \frac{d^2 y}{dt^2} = k_{\text{eff}} (g_o - y) - \epsilon_o \frac{Lw}{2y^2} V^2 - \frac{A_{132} Lw}{6\pi y^3} \] \hspace{1cm} (3.43)

To make the analysis of this system more general we need to non-dimensionalize the equation of motion. This is accomplished by first examining the SI units of key parameters in equation 3.43 to find the fundamental units.
\[ [m] = kg \]
\[ [g, g_0] = m \]
\[ [k_{eff}] = \frac{kg}{s^2} \]
\[ [\epsilon_o] = \frac{s^4 A^2}{m^3 kg} \]
\[ [A_{132}] = \frac{m^2 kg}{s^4 A} \]
\[ [V] = \frac{m^2 kg}{s^4 A} \]

From this the fundamental units are identified as: kg, m, s, and A. Next by using the Buckingham Pi theorem the following non-dimensional system parameter are constructed. Here we note that the parameter \( \alpha \) is a function of the Hamaker constant, and \( \beta \) is a function of the applied potential. Thus \( \alpha \) is dependent on the material system and the environment that the device is operated in, and \( \beta \) may be time-dependent depending on how the device is actuated.

\[
\tau = t/T \\
M = \frac{m}{k_{eff} T} \\
u = \frac{y}{g_0} \\
\beta = \frac{\epsilon_o \ell w V^2}{k_{eff} g_0^2} \\
\alpha = \frac{A_{132} \ell w}{k_{eff} g_0^2} \tag{3.44}
\]

Finally the non-dimensional system parameters are used to non-dimensionalize the equation of motion leading to equation 3.45.

\[
M \frac{d^2 u}{d\tau^2} = 1 - u - \frac{\beta}{2u^2} - \frac{\alpha}{6\pi u^3} \tag{3.45}
\]

The non-dimensional equation of motion is general and equally applicable to electromechanically actuated switches for all scales where continuum assumptions are valid. Furthermore, by studying the non-dimensionalized equation of motion we will develop a general understanding of the system dynamics and stability and their dependence on scale.
Thus the following static and dynamical analysis will be conducted using this form of the equation of motion.

3.4.2 Analysis of the Static System

First we shall examine the static or quasi-static system. Therefore in equation 3.45 we set $M \frac{d^2 u}{d\tau^2} = 0$. We define the sum of all static forces as the function $f(u, \alpha, \beta)$, equation 3.46.

\[
f(u, \alpha, \beta) = 1 - u - \frac{\beta}{2u^2} - \frac{\alpha}{6\pi u^3} = 0 \quad (3.46)
\]

\[
\rightarrow \alpha + 6\pi u^3(2 - 3u)(1 - u) = 0 \quad (3.47)
\]

Taking the first partial of $f(u, \alpha, \beta)$ with respect to $u$ and setting it equal to 0 we have,

\[
\frac{\partial f(u, \alpha, \beta)}{\partial u} = \beta - 6u_P^2(1 - u_P) + 2u_P^3 = 0 \quad (3.48)
\]

Next, we solve equation 3.48 for $\beta$ as a function of the critical gap height $u_P$,

\[
\beta = 2(3u_P^2 - 4u_P^3) \quad (3.49)
\]

Next, using equation 3.49 with equation 3.46 we can thus solve for $\alpha$ as a function of $u_P$,

\[
\alpha = 6\pi u_P^3(3u_P - 2) \quad (3.50)
\]

If the contribution of the van der Waal’s force is neglected, then $\alpha = 0$, and from equations 3.49 and 3.50 we calculate the critical parameters $u_o = 2/3$ and $\beta_o = 8/27$, which are exactly the critical parameters typically calculated for MEMS and NEMS systems when the van der Waals force is neglected [142]. These values are boxed in figures 3.23 and 3.22.
Now, using 2nd order perturbation theory we can solve equation 3.50, which is non-linear, for an approximate analytic expression of the critical pull-in gap as a function of $\alpha$, given by equation 3.51. Using this equation with equation 3.49 we can approximate the dependence of $\beta$ on $\alpha$, which is given by equation 3.52.

$$\ddot{u} = u_o + \frac{3}{16\pi} \alpha$$ (3.51)

$$\dot{\beta} = \frac{6\pi \dddot{u} (1 - \ddot{u}) - \alpha}{3\pi \ddot{u}}$$ (3.52)

The variation of $u_{PI}$ with $\alpha$ and of $\beta$ with $\alpha$ have been plotted in figures 3.23 and 3.22. In the following plots the critical value $\alpha = \alpha^* \approx 2$ has been marked by a star. As is seen in figure 3.22, $a = \alpha^*$ is defined as the value of $\alpha$ at $\beta = 0$. Now, $\beta$ is dependent on the applied voltage, thus $\beta = 0$ corresponds to a zero applied potential. Thus at $u(\alpha^*)$ a device with zero applied potential will snap down, thus failing due to stiction. We see from figure 3.23 that for $\alpha = \alpha^*$ this pull-in phenomena occurs at $u_{PI} \approx 0.75g_o$. Therefore it follows that if van der Waals forces are large enough a device can fail prior to application of an electrostatic load. If the van der Waals forces are significant, but not significant enough to cause failure, the resulting static displacement may substantially lower the pull-in voltage.

### 3.4.3 Analysis of the Non-Linear System Dynamics

Here the analysis of the non-linear system dynamics will be accomplished by examining bifurcation diagrams and phase plots for varying system parameters. Bifurcation diagrams of the variation of $u$ with $\beta$ for varying values of $\alpha > \alpha^*$, and of the variation of $u$ with $\alpha$ for varying values of $\beta > 0$, have been plotted and are shown below in figures 3.24 and 3.25. The following plots diagrams illustrate the non-linear interplay of the van der Waals force and the electrostatic force, and will be used to aid in the proceeding stability analysis of equilibrium points.
3.4.3.1 Stability of Equilibrium Points

To analyze the system stability and solve 3.45, we must first cast the equation which is a second order ordinary differential equation (ODE) as a system of first order ODEs, equation set 3.55. The stability of the system can then be studied via the Eigen values of the Jacobian matrix, and the system of first order ODEs solved using a numerical ODE.
Figure 3.24: Bifurcation diagram for Displacement Vs. $\beta$ for varying values of $\alpha$

To cast the equation of motion as a system of first order ODEs we first define the variables,

$$
x_1 = u
$$

$$
x_2 = u' \tag{3.53}
$$

Figure 3.25: Bifurcation diagram for Displacement Vs. $\alpha$ for varying values of $\beta$
and take their derivatives with respect to time,

\[ x'_1 = u' \]
\[ x'_2 = u'' \] (3.54)

It follows from application of equation 3.45 and the definitions of the defined variables \( x_1 \) and \( x_2 \),

\[ x'_1 = x_2 \]
\[ x'_2 = 1 - x_1 - \frac{\beta}{2x_1} - \frac{\alpha}{6\pi x_1^3} \] (3.55)

To this end we have cast the second order equation of motion as a set of first order ODEs now dependent on variables \( x_1 \) and \( x_2 \), which are defined as the non-dimensional displacement and velocity respectively.

To analyze the stability of this system we need to calculate the system Jacobian equation 3.56, and solve the characteristic equation, 3.60, for the Eigen values [26]. The Jacobian is calculated as follows:

\[
J = \begin{bmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\
\frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2}
\end{bmatrix}
\] (3.56)

\[
\rightarrow J = \begin{bmatrix}
0 & 1 \\
\frac{\beta}{u^3} + \frac{\alpha}{2\pi u^4} - 1 & 0
\end{bmatrix}
\] (3.57)

\[
det(J - \lambda I) \rightarrow \lambda^2 = \frac{\beta}{u^3} + \frac{\alpha}{2\pi u^4} - 1
\] (3.58)

Here we will analyze the system’s stability for the case \( \beta = 0 \), which corresponds to the case where we have a zero applied bias, but the following analysis could be conducted for any feasible system parameter. Now, for \( \alpha < \alpha^* \) and \( \beta > 0 \) there exist 2 unique stability points \( \exists u_1 > u_{PL} > u_2 \). This statement is illustrated in the bifurcation diagram of \( u \) versus \( \beta \) for varying values of \( \alpha > \alpha^* \), figure 3.24. There the stability points \( u_1 \) and \( u_2 \) have been
circled in green for different values of $\alpha$. It is interesting to note that for the special case $\alpha = \alpha^*$ there exists no stable points but only the critical point $u_{PI} = u_0$, which again has been boxed for clarity.

For the case $u_1 > u_{PI}$ we have from equation 3.60,

$$\det(J - \lambda I)\lambda^2 = \frac{\alpha}{2\pi u_1^4} - 1 < 0$$  \hspace{1cm} (3.59)

For $\beta = 0$, $\alpha < \alpha^*$, and $u_1 > u_{PI}$, the stability point $u_1$ produces a pair of purely imaginary Eigen values, $\lambda_1 = -\lambda_2$. By definition $u_1$ is therefore an Hopf point [26]. The Hopf point is identified in a phase plots as a point surrounded by periodic orbits. Hopf points are seen in figures 3.26 and 3.27.

For the case $u_2 < u_{PI}$ we have from equation 3.60,

$$\det(J - \lambda I)\lambda^2 = \frac{\alpha}{2\pi u_2^4} - 1 > 0$$  \hspace{1cm} (3.60)

For $\beta = 0$, $\alpha < \alpha^*$, and $u_2 < u_{PI}$, the stability point $u_2$ produces a pair of Eigen values, $\lambda_1 = -\lambda_2$, existing strictly in the set of real numbers. By definition $u_2$ is therefore an unstable saddle point [26]. The unstable saddle point marks the boundary in the phase plane where the unstable solution set meets the stable solution set. This point can also be identified by finding the homoclinic orbit. This special orbit is defined as the trajectory of a dynamical system that joins an equilibrium saddle point to itself. This orbit is therefore distinct from the periodic trajectories that are seen to orbit the Hopf point because it actually passes through the saddle point. These orbits are seen in figures 3.26 and 3.27.

### 3.4.3.2 Phase Diagrams

Phase plots of the system for $\alpha = 1$ and varying values of $\beta > 0$ are shown below in figures 3.26-3.29. Several interesting features of the MEMS/NEMS system described by this section are elucidated in these plots. The first plot is of the system for $\beta = 0$, the zero
applied potential case as described above. We note that a fairly large stability region exists, depending on the initial conditions. However if the system was sufficiently excited, say by thermally induced vibrations, it would quickly fall into the unstable region which would result in pull-in and failure of the device. This is shown by the outer most trajectories that surround the stable orbits of the Hopf point.

In the second plot $\beta$ has been increased to a value of 0.1. This describes the application of some potential to the system. The effect of this increase in applied potential is clearly evident in Figure 3.27. As compared to 3.26, we see that the area of stable region has been significantly reduced, and the area of the unstable region increased as the unstable saddle point and the Hopf point have begun to converge. This convergence can also be seen in bifurcation diagram of $u$ versus $\beta$. As $\beta$ increases, $\Delta u$ between the equilibrium points decreases. The decrease in the area of the stability region implies that for an even smaller perturbation in displacement or velocity the device will become unstable, resulting in pull-in of the device.

Finally, in figures 3.28 and 3.29 $\beta$ has been increased to a value of 0.2 and 0.25 respectively. In these plots we see that by further increasing the applied potential we have effectively removed all stability points from the system. Therefore for these parameters of $\alpha$ and $\beta$ we would expect the device to pull-in.

For the sake of a comprehensive comparison the phase plots for $\alpha = 0$ and varying values of $\beta > 0$ are shown below. Again, The case $\alpha = 0$ corresponds to a system with negligible van der Waals interaction. In figure 3.30 $\beta = 0$, the zero bias case. Here we see that for negligible van der Waals interaction the system is completely stable with only a Hopf point and no saddle point as was the case for $\alpha = 1$. This is to be expected because the instability for the zero bias case can only be introduced by some external force acting on the system, and if there is no van der Waals force there are no external forces acting on the system.

Figures 3.31-3.32 illustrate what was observed in the preceding phase plots for $\alpha = 1$
Figure 3.26: Phase diagram of the system for $\alpha = 1$ and $\beta = 0$

Figure 3.27: Phase diagram of the system for $\alpha = 1$ and $\beta = 0.1$

Figure 3.28: Phase diagram of the system for $\alpha = 1$ and $\beta = 0.2$
Figure 3.29: Phase diagram of the system for $\alpha = 0$ and $\beta = 0.25$
and \( \beta \leq 0.1 \). These phase plots show the evolution of the unstable region as the applied potential is increased. First, we see that application of a bias introduces an unstable saddle point to the phase space. Next we note that as the bias is increased, the area of the stability region decreases as the unstable and stable regions converge. Finally, in figure 3.33 \( \beta \) has been increased to a value of 0.5, and we see that the Hopf point and unstable saddle point have been completely removed, implying that the system has become completely unstable resulting in pull-in of the device.

3.4.4 van der Waals Detachment Length

From the preceding analyses we can calculate the detachment length of a given system. The detachment length of a system is defined as the maximum length that a suspended and non-biased membrane can have before the van der Waals force dominates the restoring force of the membrane, thereby causing the membrane to collapse to the substrate. It is obvious that for properly function MEMS/NEMS devices this scenario must be avoided. Thus the detachment should be used as a design parameter for systems with gaps < 100 nm.

From the dimensionless parameter \( \alpha \) we have,

\[
\alpha = \frac{A_{132}Lw}{k_{eff}g_0^4}
\]  

(3.61)

and considering the effective stiffnesses of two types of devices that have been considered in this thesis, the cantilever, and fixed-fixed beam, but subjected to a distributed load,

Cantilever [17]:

\[
k_{eff} = \frac{8EI}{L^3}
\]

(3.62)

Fixed-Fixed Beam 3.23:

\[
k_{eff} = \frac{384EI}{L^3}
\]

(3.63)

The detachment lengths are derived by evaluating equation 3.61 at \( \alpha^* \approx 2 \).
Figure 3.30: Phase diagram of the system for $\alpha = 0$ and $\beta = 0$
Figure 3.31: Phase diagram of the system for $\alpha = 0$ and $\beta = 0.1$

Figure 3.32: Phase diagram of the system for $\alpha = 0$ and $\beta = 0.25$
Figure 3.33: Phase diagram of the system for $\alpha = 0$ and $\beta = 0.5$
3.4.4.1 Device: Cantilever

Inserting equation 3.62 into equation 3.61 evaluated at $\alpha^*$ we have,

$$\alpha^* \frac{8EI}{l_{\text{detach}}} g_0^4 = A_{132} l_{\text{detach}} w$$

$$\rightarrow l_{\text{detach}} = \sqrt[4]{\frac{2\alpha^* E l^3}{3A_{132}}} g_0^3$$

(3.64)

3.4.4.2 Device: Fixed-Fixed Beam

Inserting equation 3.63 into equation 3.61 evaluated at $\alpha^*$ we have,

$$\alpha^* \frac{384EI}{l_{\text{detach}}} g_0^4 = A_{132} l_{\text{detach}} w$$

$$\rightarrow l_{\text{detach}} = \sqrt[4]{\frac{32\alpha^* E l^3}{3A_{132}}} g_0^3$$

(3.65)

From equations 3.64 and 3.65 we see that the detachment length is linearly proportional to the initial gap height, $g_0$. This is different from the relationship of detachment length to initial gap height when the Casimir force is considered instead of the van der Waals force [142], which is instead proportional to $g_0^{3/2}$. Detachment curves for feasible fixed-fixed and cantilever type WALD NEMS switches are given in figure 3.34. It should be noted that for all gap heights the detachment length of cantilever devices is less than that of fixed-fixed devices. This makes sense because fixed-fixed structures are inherently stiffer than a cantilever structure of the same length due to their additional support.

3.5 Tunneling Current

During pull-in characterization of the 50 nm generation of WALD switches, chapter 6 section 5.3, it was frequently observed that low levels of current < 20 nA were measured for applied biases < 3 Volts, and that in this region the IV curves shared a striking resemblance to IV curves used to characterize MEMS tunneling accelerometers [129, 48, 85]. Lee et al more recently attributed the non-linear increase in measured current during characterization of their CNT devices to tunneling behavior induced as the device is drawn towards the actuation electrode [135]. The techniques for characterization of MEMS/ NEMS tunneling
Figure 3.34: $l_{\text{detach}}$ Vs. $g_a$ for rectangular WALD NEMS systems; the detachment length for cantilever type devices is plotted in blue; the detachment length for fixed-fixed type devices is plotted in black; system parameters: $E = 400$ GPa, $t = 30$ nm, $w = 500$ nm, $A_{132} = 22 \times 10^{-20} m^2 kgs^{-2}$
barrier heights presented in this section represent a great improvement upon those presented elsewhere [48, 85].

### 3.5.1 Electron Tunneling

Tunneling current is a quantum phenomenon that results from the dualistic wave-particle nature of matter, in this case electrons. Tunneling can be understood by considering energy levels of electrons within our device. First we consider a particle within the tungsten that is drawn to the surface of the device by the electric field when a voltage difference is applied. This electron will have an associated energy, and proportional to that energy an associated de Broglie wavelength, figure 3.35, left side of plot. Now, the gap between the WALD bridge structure and Au actuation electrode represents an energy barrier between the two materials. The height of the barrier corresponds to the energy required for an electron to leave the tungsten lattice and become a free-electron, and the difference between the potential "height" and electrons energy is defined as the work function. Thus, the work function is the amount of energy that must be given to an electron to free it from its material.

Solutions to Schrödinger's equation, equation 3.66, yield the wave function of an electron in a given region. For example, figure 3.35 has three regions: one to the left of the barrier (our WALD device), the barrier (the energy needed to free an electron from the WALD), and the region to the right of the barrier (free space). Solutions to Schrödinger's equation are shown in the bottom plot of figure 3.35. Thus we see that within the barrier the electron’s wave function decreases exponentially.

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}, t) + V(\vec{r}, t)\Psi(\vec{r}, t)$$ (3.66)

Coupled with the wave function of the electron is the probability of the location of the electron at any given moment – a result of the Heisenberg uncertainty principle. Classically we do not expect an electron to penetrate the barrier; however, because the electron’s position
Figure 3.35: (a) Model of an electron in a square energy well with a given energy; (b) associated wave function for the electron as it approaches and tunnels through the potential barrier [125].

is based on a probability instead of a known position, if the barrier width is sufficiently small there will exist some probability that the electron does in fact exist across the barrier. If this is the case, the electron is said to have tunneled through the barrier. The rate in time at which this occurs is the tunneling current [69, 210].

3.5.2 Field Emission Current Density

Typically the energy of and position of electrons confined to a metal are described by solving the 1-D Schrödinger time-independent equation for a square potential barrier. However in the presence of a strong electric field the potential is best represented by a triangular barrier whose shape is dependent on the magnitude of the applied field, equation 3.67. In figure 3.36 is a qualitative illustration of two energy wells separated by a triangular
barrier, and a square barrier—highlighted in red.

In figure 3.36 an electron with energy $E$ approaches the potential barrier from the left. For the energy level illustrated the triangular barrier width $L$ is significantly less than for the zero-biased case, which is represented by the square barrier. The slope of the triangular potential barrier is determined by the magnitude of the electric field, thus as we see in the figure the effect of increasing the strength of the electric field is to decrease the effective width of the potential barrier for all energy levels. Therefore, it follows that the probability of tunneling for an electron with energy $E$ can be greatly increased by application of a significantly strong electric field to the surface of a metal. This phenomenon is called field emission and is discussed in detail in [69].

As a historical note, Gerd Binnig and Heinrich Rohrer developed the scanning tunneling microscope (STM) in 1981 while working for IBM Zurich. In brief, images are constructed based on variations in tunneling current as a tungsten probe is scanned above the surface of a sample. The instrument is capable of producing images with atomic level resolution

$$V(x) = V_o - \sqrt{E \cdot E} x$$  \hspace{1cm} (3.67)

The solution to the 1-D time-independent Schrödinger equation for a triangular barrier will not be discussed in detail here, but if the reader is interested an excellent comprehensive derivation of the solution is given by French and Taylor in their text An Introduction to Quantum Physics. For a triangular potential barrier the transmission coefficient, which is the probability of an electron tunneling through the barrier, is given by equation 3.68 [69]. The transmission coefficient, and therefore tunneling current, is dependent on $E_f$, the work function of the material, which is defined as the minimum energy needed to remove an electron from a solid into vacuum, as well as $\sqrt{E \cdot E}$, the magnitude of the applied electric field.

$$T = e^{-\frac{4}{3} \frac{\sqrt{2m_e \hbar}}{\sqrt{2m_e \hbar}}} E_f^{3/2}$$  \hspace{1cm} (3.68)
Figure 3.36: Energy well for field emission; In the presence of a large electric field the potential barrier is modeled by a triangular barrier whose slope is proportional to the electric field strength.

To calculate the current density the transmission coefficient can be multiplied by the coefficient $J_0$, equation 3.69. $J_0$ has the units of current per area and is given by equation 3.70. In the equation $n$ is the number of charge carriers per volume, $q$ is the carrier charge, and $v$ is the carrier velocity.

$$J = J_0 T$$ \hspace{1cm} (3.69)

$$J_0 = nqv$$ \hspace{1cm} (3.70)

Now, for a conductor the number of available carriers per volume, $n$, is dependent on the Fermi energy, $E_f$, and calculated by equations 3.71-3.74 [188]. The electron density of states, $\rho(E)$, and the Fermi-Dirac distribution function, $f_{FD}(E)$, are given by,

$$\frac{dn_e}{dE} = \rho(E) f_{FD}(E)$$ \hspace{1cm} (3.71)
\[ \rho(E) = \frac{8\sqrt{2\pi m_e^3}}{\hbar^3} \sqrt{E} \]  
\[ f_{FD}(E) = \frac{1}{e^{(E-E_f)/kT}+1} \]  

Equation (3.72)

For simplicity, if we consider that case where \( T \to 0 \) K, the density of carriers can be calculated by integrating equation 3.71 from \( E = 0 \) to \( E = E_f \), equation 3.73.

\[ n_e = \frac{8\sqrt{2\pi m_e^3}}{\hbar^3} \int_0^{E_f} \sqrt{E} dE \]  
\[ (3.73) \]

Evaluating the integral we arrive at equation 3.74, which allows us to calculate the volumetric density of free carriers for a known fermi-energy.

\[ n_e = \frac{16\sqrt{2\pi m_e^3}}{3\hbar^3} E_f^{3/2} \]  
\[ (3.74) \]

Next, the velocity of the electron is calculated by assuming that the electron’s kinetic energy is equal to that of the fermi energy \( E_f \), equation 3.75. This velocity is sometimes called the fermi velocity.

\[ v_e = \sqrt{\frac{2q_e E_f}{m_e}} \]  
\[ (3.75) \]

By evaluating equations 3.71-3.75, the tunneling current coefficient \( J_o \) given by equation 3.70 can be calculated. To calculate the tunneling current density the only thing left to do is evaluate equation 3.68 to calculate the transmission coefficient.

### 3.5.3 Approximation of Electric Field Strength at Thin-Film Corners

The transmission coefficient, given by 3.68, is dependent on the magnitude of the applied electric field. Significant tunneling typically occurs for field strengths greater than \( 10^8 \) V/m. If a parallel plate model is assumed, where the electric field is given by \( V/g \), the approximated pre-actuation electric fields for a typical MEMS/NEMS switch are not large enough to induce the magnitude of tunneling current that has been measured and reported.
STM microscopes work because the STM probe is exactly 1 W atom sharp, thus at the tip of the probe the electric field is approximately \( V/r_W \), resulting in very large electric fields at the tip which in turn induce appreciable tunneling current for small biases.

Now, it is well known that the magnitude of electric field is greatly increased by sharp geometric features, which implies that the electric field surrounding a biased structure having a rectangular structure should be greatest at the corners. The field at the corners is called the fringe field, and is largely neglected in the modeling of MEMS and NEMS electrostatically actuated devices. Based on previously reported IV characterization of MEMS and NEMS devices, IV characterization of various WALD devices conducted by this research effort, and STM theory, it is hypothesized that the tunneling current measured for MEMS/NEMS devices with rectangular cross-sections is induced by the electric field at the corners of the biased structure. It is therefore the goal of this section to develop an empirical equation derived from numerical experiments which adequately approximates the maximum magnitude of an electric field acting on a biased rectangular structure.

The empirical equation will be derived by assuming that the total electric field \( E_\Sigma \) is the sum of a parallel plate contribution \( E_\parallel \), and a corner contribution \( E_C \), equation 3.76.

\[
E_\Sigma = E_\parallel + E_C
\]

\[
E_\parallel = \frac{V}{g}
\]

\[
E_\Sigma = \sqrt{E \cdot E}
\]

where \( g \) is the gap height at the point of maximum deflection,

\[
g = g_o - y
\] (3.77)

In this way if the magnitude of the electric field at the corner of a biased rectangular structure is known, the contribution to the electric field by the corner can be calculated by simply subtracting the parallel plate contribution from the total electric field, equation 3.78.
\[ E_C = \sqrt{\mathbf{E} \cdot \mathbf{E}} - \frac{V}{g} \]  

(3.78)

3.5.3.1 Experimental Procedure

Quantum theory tells us that tunneling should occur at the place where tunneling is most probable. Therefore one would only expect tunneling to most likely occur at some region corresponding to the location of the electric field maximum. Because the field is inversely proportional to the separation distance between conductors, the maximum of the electric field is expected to coincide with the point of maximum deflection of an electrostatically actuated switch. Hence, for a fixed-fixed device the maximum of the electric field is expected to occur at approximately \( x = L/2 \), and for a cantilever beam at \( x = L \), where \( L \) is the beam length. For this reason the electric field around the rest of the device can be neglected, which implies that a 2-D model of the device geometry at the point of maximum deflection is sufficient to study the electric field acting on a biased rectangular structure. A schematic of the of the model geometry is illustrated in figure 3.37.

For the following study, a 2-D FEM model was developed using COMSOL Multiphysics to solve Laplace’s equation for the potential and associated electric field resulting from a bias applied across a conducting plane and a suspended conductor. For simplicity the medium between the conductors was modeled using a relative electrical permittivity of 1. To accurately calculate the electric field surrounding the suspended structure, a domain much larger than the suspended structure was meshed, with the mesh finely refined around the structure. A voltage \( V_{GS} \) was applied to the bottom boundary of the domain, and the suspended structure (source) grounded. The model was biased in this way because this is how the WALD devices developed by this work were typically biased. Finally, a zero charge boundary condition was applied to the left, right, and top boundaries of the domain. Figure 3.38a shows a surface plot of \( E_y \), and 3.38b shows a surface plot of \( E_x \), with \( E \) represented by stream lines in both figures. The plots were generated for a model having with following
parameters: \( w = 500 \text{ nm}, \ t = 128 \text{ nm}, \ g = 250 \text{ nm}, \) and \( V_{GS} = 1 \text{ V} \). The white region is the area of space occupied by suspended conductor, and as expected the maximum of the electric field, highlighted in red, is located at the structure corners nearest to the conducting plane across which the potential has been applied.

Figure 3.37: Illustration of a deflected fixed-fixed thin-film NEMS switch and cross-section taken at the point of maximum deflection \( x = L/2 \)

Figure 3.38: FEM calculated electric field around a rectangular conductor; (a) surface plot of \( E_y \); (b) surface plot of \( E_x \); In both figures \( \mathbf{E} \) is represented by stream lines; The electric field maximum is found at the corners and is highlighted in red

To investigate the corner’s contribution to the electric field the thickness, gap height,
and applied bias were varied and the electric field calculated. The maximum of the electric field was calculated by $E_{\parallel} = \sqrt{E \cdot E_{\text{max}}}$ and the parallel plate contribution extracted using equation 3.78. This procedure was repeated for various voltages, and plots of $E_C$ versus gap height were generated, figures 3.39a-c. The investigated geometric parameters, i.e., thickness, gap height and width, were all chosen to typical reflect thin-film NEMS dimensions. Specifically, $t = 32 \text{ nm}$ was chosen because it is the thickness of WALD used as the structural material for every device that was developed by this research effort. Finally, applied voltages were chosen such that $0.5 \leq V_{GS} \leq 3 \text{ V}$, which accurately represent the operating voltages of reported NEMS devices and WALD NEMS switches developed here.

3.5.3.2 Results

In figures 3.39a-c $E_C$ has been plotted as a function of gap height for varying thicknesses and applied potentials. For every set of plots the data were best fit by the power law, $E_C = \kappa g^{-\beta}$. Furthermore, because the thickness of the suspended conductor and the potential were varied, the dependency of the power law coefficients $\kappa$ and $\beta$ on specific model parameters is immediately evident. Comparing figures 3.39a-c it is seen that the power coefficient $\beta$ varies with thickness, but remains constant for all applied voltages; on the other hand, the coefficient $\kappa$ varies for both thickness and applied voltage. Thus from this initial study we know that $E_C$ is dependent on applied voltage, structure thickness, and gap gap height, and is of the form given by equation 3.79.

$$E_C = \kappa(t, V)g^{-\beta(t)}$$  \hspace{1cm} (3.79)

3.5.3.3 Study of Power Law Coefficients $\kappa$ and $\beta$

The dependence of $\beta$ on film-thickness has been plotted in figure 3.40 using the values extracted from figures 3.39a-c, which are listed in table 3.2. The plot revealed a strong linear relationship between $\beta$ and thin-film thickness with $R^2 \approx 0.96$. The equation of the best fit
Figure 3.39: Electric-field study: $E_C$ Vs. Gap Height; Model geometries: $w = 500$ nm, $t = \{8, 32, 128\}$ nm; Experiments conducted for $V_{GS} = \{0.5, 1, 3\}$ Volts (figures a, b, c)
line is given by below by equation 3.80.

\[ \beta(t) = 2 \times 10^6 t - 0.384 \]  \hspace{1cm} (3.80)

To derive an expression for the power law parameter \( \kappa \) it was assumed via separation of variables that the parameter \( \kappa(t,V) \) was the product of two functions \( \alpha_1(t) \) and \( \alpha_2(V) \). This assumption allowed \( \kappa \) to be studied by varying one variable at a time and plotting \( \kappa \) as a function of that variable. In the plot shown in figure 3.41, \( \kappa \) was plotted as a function of applied voltage for a thickness of 8, 32, and 64 nm. From this study the parameter \( \kappa \) was found to be linearly dependent on the applied voltage, with \( R^2 = \{ .998, 1, 1 \} \) corresponding
to the respective thicknesses. Therefore, $\alpha_2 = V_{GS} = V$, and $\kappa(t, V) = \alpha_1(t)V$.

![k Vs. VGS](image1)

Figure 3.41: $\kappa$ Vs. $V_{GS}$; Model geometry: 500 x 32 nm, $g = 250$ nm

Next, the parameter $\alpha_1$ was derived by plotting the linear coefficients found in figure 3.41 as a function of thickness for $V_{GS} = 1$ V, figure 3.42. These values are listed in table 3.3. By fitting the data from this set it was found that the parameter $\alpha_1$ is exponentially dependent on the thin-film thickness, equation 3.81.

![a1 Vs. Thin-film Thickness: VGS = 1 V](image2)

Figure 3.42: $\alpha_1$ Vs. Thin-film Thickness; Model geometry: $w = 500$ nm; $V_{GS} = 1$ Volt
Table 3.3: $\alpha_1$ Vs. Thin-film Thickness

<table>
<thead>
<tr>
<th>thickness [nm]</th>
<th>$\alpha_1(t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>83,880</td>
</tr>
<tr>
<td>32</td>
<td>11,532</td>
</tr>
<tr>
<td>128</td>
<td>663.79</td>
</tr>
</tbody>
</table>

$\alpha_1(t) = 119,306e^{-40 \times 10^6 t}$  \hspace{1cm} (3.81)

Therefore, assuming separation of variables $\kappa(t, V)$ is given by equation 3.82.

$\kappa(t, V) = 119,306Ve^{-40 \times 10^6 t}$  \hspace{1cm} (3.82)

Thus far all model parameters have been considered except for the structure width. To study any possible dependency of the electric field on width, the electric field was calculated for varying width while holding the parameters $t$, $g$, $w$, and $V$ constant. For this study the model parameters were as follows: $t = 32$ nm, $g = 250$ nm, $V_{GS} = 1$ V. The results of this study are plotted in figure 3.43.

Figure 3.43: $\alpha_1$ Vs. thin-film thickness; Model geometry: $w = 500$ nm; $V_{GS} = 1$ Volt
In figure 3.43 the maximum of the electric field is plotted as a function of width. Also, the average of the maximum of the calculated field strength for all investigated widths is plotted along with error bars representing ±1 standard deviation. It is seen that the calculated electric field values are nearly constant in width, with most of the calculated values falling within one standard deviation. The reason that some values do not fall within 1 standard deviation is most likely due to variation in mesh refinement. It is therefore concluded that the maximum of the electric field, located at the structure corners closest to the substrate, is independent of structure width. This implies that the maximum electric field for a thin-film structure having any feasible piece-wise and smooth profile may be calculated using the derived equations. In the scope of this research this means that these equations are equally applicable to rectangular, bow-tie, and poly-tie WALD devices. Therefore, using equations 3.80 and 3.82 with equation 3.79, \( E_C \) is given by equation 3.83.

\[
E_C(g, t, V) = 119,306V e^{-40 \times 10^6 t} g^{-\left(2 \times 10^6 t + 0.384\right)} 
\]  

(3.83)

### 3.5.3.4 Correction Factor

Finally, to verify the validity of the derived equations, \( E_{\Sigma, max} \) was calculated for several randomly chosen models using the FEM model and equation 3.76. It was observed that the % difference error between the two methods was consistently around ±20%. As is often times the case for empirical equations derived via numerical experiments, a correction factor \( 0 < \Theta \leq 1 \) which multiplies equation 3.76 has been introduced to minimize error between FEM and analytically calculated values of \( E_{\Sigma, max} \). It was found that for \( \Theta = 0.8 \) the error between field strengths calculated via FEM, and those using equation 3.84, can be bound between approximately ±5%. Including the correction factor \( \Theta \), the maximum of the total electric field acting on a biased rectangular conductor, including fringe-field/corner contributions, is therefore given by equation 3.84.
\[ E_{\Sigma}(g, t, V)_{\text{max}} = \Theta \left( \frac{V}{g_o - y} + 119, 306 Ve^{-40 \times 10^6 t} (g_o - y)^{-\left(2 \times 10^6 t + 0.384\right)} \right) \] (3.84)

### 3.5.4 Extended Field Emission/Tunneling Current Model For MEMS/NEMS Electrostatically Actuated Devices

For a MEMS/NEMS electrostatically actuated switch the maximum field strength, and therefore tunneling current, can thus be approximated for any applied voltage by using 3.84 with the expression or current density, equation 3.69. For a MEMS/NEMS device the tunneling current density is dependent on the gap height, which itself a function of applied voltage. Unfortunately the relationship between gap height and applied bias is non-linear, and therefore no closed-form solutions exist. The displacement of MEMS/NEMS switch for a given voltage \( V \) can be calculated via a linear approximation such as the one given by equation 3.85, but for a more accurate approximation the displacement should be calculated using numerical methods, such as those presented in chapter 4. In equation 3.85 \( \epsilon_o \) is the permeability of free space, \( A \) is the area over which the electrostatic load is distributed, \( k_{eff} \) is the effective stiffness of the device, \( g_o \) is the initial gap height, and \( V \) the applied potential.

\[ y_{\text{linear}} \approx \sqrt{\frac{\epsilon_o A}{2k_{eff}g_o}V} \] (3.85)

As an example, the displacement versus applied voltage for a 2-terminal WALD NEMS switch with dimensions: 4,000 x 500 x 32 nm and \( g_o = 50 \) nm, calculated via equation 3.85 and the multi-physics FEM described buy chapter 4 have been plotted in figure 3.44. It is seen that the linear approximation given by equation 3.85 overestimates the FEM displacement for all \( V_{GS} \), with the maximum difference between the two somewhere near \( V_{GS} \approx 2/3V_{\text{pullin}} \), and this is true for all approximations regardless of geometry.

The tunneling current is calculated by multiplying the current density by the area bounding the flux of tunneling electrons. The tip of an STM probe is electrochemically
etched such that it is ideally 1 W atom sharp. Thus the electric field magnitude and tunneling current probability are greatest at the tip of the probe, therefore the flux of tunneling electrons passes through an area defined by the tip radius. For thin-film devices with multiple edges it is feasible that several atomic sites may have similar transmission probabilities, and hence each site might contribute an appreciable amount of current to the total tunneling current. Thus it is reasoned that the area used to calculate the tunneling current for a MEMS/NEMS device should be some integer multiple ($\gamma$) of the atomic radius ($r_{a-}$) of the negatively charged structure. Finally, the barrier height’s extracted when characterizing MEMS tunneling devices are commonly an order of magnitude less than the work function of the device material. For this reason $E_f$ in equations 3.68-3.75 is replaced by the parameter $\phi$ which is defined as the effective barrier height. The field emitted tunneling current for a MEMS/NEMS device is therefore given by equation 3.86.

$$I = J_o \exp \left( \frac{-4\sqrt{2m_e}}{3hq_e \Theta \left( \frac{V}{g_o - y} + 119,306V e^{-40 \times 10^6 t (g_o - y)} \right)^{(2 \times 10^6 t + 0.384)/3}} \right) \left( \gamma \pi r_{a-}^2 \right) \phi^{3/2} \right)$$ (3.86)

with the coefficient $J_o$ is explicitly given by,
\[ J_o = q_e \left( \frac{16\sqrt{2}\pi m_e^{3/2}}{3\hbar^4} \phi^{3/2} \right) \left( \sqrt{\frac{2q_e \phi}{m_e}} \right) \]

with \( q_e = 1.6022 \times 10^{-19} \) C

### 3.5.4.1 Discussion

The complete model given by equations 3.86 and 3.87 is an extension of the quantum theory of field emission that specifically considers the device physics of thin-film electromechanically actuated MEMS and NEMS devices. The model has been derived starting from the 1-D time-independent form of Schrödinger’s equation and extended for thin-film MEMS/NEMS devices via a detailed numerical study of the electric field acting on a biased and suspended rectangular conducting structure. The tunneling current’s dependency on the electromechanical response of the device comes from the electric field’s dependency on gap height, and therefore the electrostatically induced displacement of the device. The electromechanical aspect of this problem can be sufficiently handled using analytic models for pull-in as derived in section 3.2, or by means of the FEM model described by chapter 4 and given in appendix F.

Previously measured tunneling current in MEMS/NEMS devices was characterized using basic tunneling theory derived from the 1-D Schrödinger’s equation applied to a square barrier. As such, these models neglected the quantum tunneling effects which result from field emission. Furthermore, the theory used to characterize tunneling current was only useful for extracting the effective barrier height, as will be seen in chapter 6 section 6.4, and is not able to predict pre-actuation tunneling IV curves. By contrast, the model developed here considers field emission, and electric field effects, can be used for device characterization, and to predict pre-actuation tunneling IV curves.
3.5.5 Theoretical Case studies

Using the developed model a theoretical case study has been conducted. For the study two different 2-terminal WALD NEMS switches were considered. The chosen dimensions for the WALD structure for both devices was 4,000 x 500 x 32 nm, with a gate-to-source overlap of 100%. For one model a gate-to-source gap height of 50 nm was chosen, and for the other a gap height of 15 nm. As a result of the different gap heights \( V_{\text{pullin}} = \{3.4, 0.56\} \) respectively. The disparity in gap heights and associated pull-in voltages allows us to study the dependency of tunneling current on gap height and applied voltage, which is of some value as the critical dimensions of NEMS devices continue to decrease.

For the study, tunneling current versus applied voltage for the devices described has been calculated for varying \( \phi \) using the developed model. The tunneling current has been calculated for device displacements approximated using the FEM software given in appendix F and via the linear approximation given by equation 3.85. Finally, the error between FEM and linearly approximated tunneling current for varying \( \phi \) has been studied.

3.5.5.1 Variation of \( \phi \)

For MEMS tunneling devices having a similar material system to that modeled here, an effective barrier height \( 0.05 \leq \phi \leq 0.055 \) eV is typically extracted via STM theory [48, 85, 129]. For this reason only values of \( \phi \) in this range have been considered in the following study. The FEM model given in appendix F was used to calculate displacement versus applied voltage for the devices described. To calculate the pre-exponential coefficient \( J_0 \), equation 3.69, the Fermi-energy \( E_f \) has been replaced by \( 0.05 \leq \phi \leq 0.055 \). Results for the 50 and 15 nm devices are given in figures 3.45 and 3.46 respectively.

For the 50 nm gap it is seen that for \( \phi \leq 0.9 \) eV the IV curves bend, becoming nearly linear as \( V_{\text{GS}} \) increases. However, for the 15 nm gap the IV curves remain exponential. Work functions in this range are typical for MEMS tunneling devices operated in air with
appreciable surface contamination, i.e., oxides, water, organic contaminants etc. [48, 85, 129, 54]. This suggests that, depending on the gate-to-source gap height, the tunneling current mechanism of devices with appreciable contamination is dominated by the pre-exponential coefficient $J_0$. For the 50 nm gap height and $\phi > 0.09$ eV, the IV curves are exponentials implying that the tunneling mechanism is still dominated by the transmission coefficient $T$, equation 3.68. For both cases, as $\phi$ approaches the reported limit 0.55 eV, which implies an ideal environment, material and surface, the tunneling current prior to snap-thru is negligible.

![Figure 3.45: Modeled tunneling current for varying $\phi$; Device Geometry: 4,000 x 500 x 32 nm; $g_o = 50$ nm; $V_{pullin} = 3.4$ V](image)

3.5.5.2 FEM Vs. Linear Approximation of Displacements

The tunneling currents plotted in figures 3.45 and 3.46 were recalculated using linearly approximated device displacements, figures 3.47 and 3.48. for all cases studied the general IV characteristics, such as shape, are preserved. It is clear from this study that the linear approximation over-estimates the tunneling current, which is to be expected because from figure 3.44 we know that the approximation overestimates displacement, which directly ef-
Figure 3.46: Modeled tunneling current for varying $\phi$; Device Geometry: 4,000 x 500 x 32 nm; $g_o = 15$ nm; $V_{pullin} = 0.56$ V

...factors the magnitude of the electric field. The error between the two methods pertaining to the characterization of real devices is investigated in chapter 6 section 6.4.

Figure 3.47: FEM Vs. Linear approximations of modeled tunneling current for varying $\phi$; Device Geometry: 4,000 x 500 x 32 nm; $g_o = 50$ nm; $V_{pullin} = 3.4$ V
3.5.5.3 Error Between FEM and Linear Approximations for Varying $\phi$

For both of the modeled devices the % difference between FEM and linearly approximated IV curves were plotted as a function of applied voltage, figures 3.49 and 3.50. Here it is seen that although IV curves generated by FEM and the given linear method are qualitatively similar, there exists a large % difference between IV curves. For both devices the maximum percent difference approaches it’s maximum as $V_{GS} \to 0$ V, with % difference displaying a transcendental arccosine-like dependence on applied voltage. In figures 3.49 and 3.50 it is observed that the error between methods increases linearly as $\phi$ approaches 0.55 eV, with the error appearing to become larger with decreasing gap height. However, it must be noted that the largest errors correspond to the smallest calculated currents, typically less than 1 nA, therefore the characterized error between FEM and linearized methods should not detour one from applying linear approximation methods to the model developed here.
Figure 3.49: Error between FEM and linear approximations of modeled tunneling current for varying $\phi$; Device Geometry: 4,000 x 500 x 32 nm; $g_o = 50$ nm; $V_{pullin} = 3.4$ V

Figure 3.50: Error between FEM and linear approximations of modeled tunneling current for varying $\phi$; Device Geometry: 4,000 x 500 x 32 nm; $g_o = 15$ nm; $V_{pullin} = 0.56$ V
Chapter 4

Computational Modeling: 2-D Multi-Physics FLFD/FEM Model for Electromechanically Actuated NEMS Switches With Aspect Ratios $< 10^{-2}$

4.1 Overview

This chapter is devoted to computational modeling of the devices specific to this thesis, and described in chapter 5. The chapter begins with a brief overview of the hybrid BEM/FEM method, which has been used to model electrostatically actuated MEMS devices since the early 1990’s [197]. The current limitations of the BEM/FEM method as applied to devices with aspect ratios of the order of $10^{-3}$ are discussed, and a different approach, well suited for thin-film NEMS devices, is derived and introduced. The derivation focuses specifically on discretization methods of both the mechanical and electric domains, and on the development of a faux-Lagrangian finite difference scheme used to solve Laplace’s equation in the electric domain. Next, the implicit-explicit non-linear integration scheme used to solve the discretized equation of motion for the coupled-mechanical domain is described in some detail. The chapter concludes with several case studies used to validate the FEM model and demonstrate numerical capabilities of the developed software. The case studies focus on calculation of the electric field for 2 and 3-terminal rectangular domains, and on numerical calculation of displacement versus applied voltage curves for WALD NEMS switches from which pull-in voltages are extracted. Finally, via application of a van der Waals force module, the developed mechanical model is used to generate van der Waals-based detachment curves for various thin-film WALD structures.
4.2 Computational Modeling in MEMS

As seen in section 3.4.3, the response of MEMS/NEMS electrostatically actuated systems is highly non-linear. Therefore, accurate non-linear mathematical modeling becomes a very important technique for gaining physical understanding of these systems [198]. The solutions and study of non-linear systems most always requires computational methods. Simulation of electrostatically actuated MEMS devices has been conducted for almost two decades using the Boundary Element Method (BEM), also known as Boundary Integral Equations (BIE), to model the exterior electric field coupled with the finite element method (FEM) to model mechanical deformation of the structure [75, 15].

The need for a CAD system specific to MEMS was first identified at Transducers ’87 by Stephen Senturia et al [197]. The CAD tool developed was called MEMCAD. The early goal of the first MEMS CAD programs was to assist the engineering at all levels of the product development. Thus the focus was on developing a CAD system capable of simulating process design, device design, and integrated circuit analysis—this CAD methodology is still employed by Coventor.

From 1987 to 1992 several groups were active in the early development of MEMS-specific CAD programs. Koppelman worked on the OYSTER program, which concentrated on creating a 3-D solid geometric model from an integrated-circuit process description and mask data. Buser, Koide, and Sequin focused on 3-D geometric modeling specific to anisotropically etched silicon structures. And Cary and Zhang concentrated on developing an overall user interface to access different modules for simulating the mechanical behavior of specific structures, such as diaphragms [197].

In 1992 Stephen Senturia wrote that if FEM based methods were used to approximate exterior quantities (exterior to the mechanical domain), such as the electric field, then an exterior volume mesh would be required. And while meshes for interior domains are readily generated, the same was not true for exterior meshes. Furthermore, if a user were willing to
generate an exterior mesh a large number of nodes would be needed and thus the resulting system of equations would be computationally expensive [197]. As an alternative Senturia et al. developed a specialized BEM and mixed finite-element/boundary-element methods for the MIT MEM CAD system.

### 4.2.1 The Mixed FEM/BEM Method

Conventionally, the FEM is used to model the mechanical domain and the BEM to model the electrostatic domain and compute surface charge densities. This requires that the mechanical domain be discretized into nodes and elements. A finite element analysis is performed by applying the electrostatic pressure as a Neumann boundary condition of the mechanical domain. Deformations are computed and the geometry of the mechanical structure updated. Next, an electrostatic analysis is performed on the updated geometry by discretizing the surface of the conductor into boundary elements. The BEM is then used to compute the surface charge density of each boundary element. Once the elemental charges are known, the elemental electrostatic pressures can be calculated and reapplied to the mechanical domain, and the mechanical and electrostatic analysis repeated. The procedure described is a sequentially-coupled multi-physics approach, and the analysis is considered to be quasi-static.

The typical method for the coupled-domain analysis used by the dominant commercial packages, namely ANSYS and Coventor, require mesh generation, mesh compatibility, re-meshing, and interpolation of solutions between domains. Mesh generation can be costly for complex geometries, and severe mesh distortion can occur for large deformations. These distortions can lead to non-invertible stiffness matrices, and in turn unsolvable systems. In the model presented, contact boundaries are not considered, and the simulation is terminated following the snap-thru phenomenon. Because devices subjected to distributed loads typically snap-thru at displacements of \( \approx 40 \, \text{to} \, 45\% \) of the initial gap height, and the devices considered by this work have gap heights \(< 100 \text{ nm}\) with lengths of a couple of microns, the
ratio of displacement to device length is of the order of $10^{-3}$. Thus, for devices considered here, mesh distortions are of no concern.

One major hurdle of the coupled FEM/BEM approach is that often times the boundary elements do not match with the finite element mesh. This can be overcome by matching the finite element nodes on the surface of the mechanical domain to the boundary element nodes on the boundary of the electrostatic domain. However this method can quickly become computationally costly if either domain requires refinement. In the case that the FEM/BEM meshes are not matched an interpolation scheme must be developed to map the elemental charge densities/electrostatic pressures calculated by the BEM to the FEM mesh of the mechanical domain. If care is not taken these interpolation techniques can quickly become awkward and lead to significant errors [138].

Certain boundary equation integrals (BEIs) require special care for regions with extremely small aspect ratios. For mechanical domain this implies thin plates/shells, and for the electrostatic domain this implies gaps between conductors that are much smaller than the length of the domain. The usual BEMs deal with weakly singular, and nearly weakly singular integrals, but for domains having small aspect ratios the integrals considered are typically nearly weakly, nearly strongly, weakly, and strongly singular integrals [15]. The numerical computation of these integrals requires highly specialized, computationally expensive, and often complex integration schemes.

4.3 Euler-Lagrange FE Formulation of the Mechanical Domain

The discretized governing equation of motion for the mechanical domain is derived here. There are several approaches commonly used in derivation and discretization of governing equations, such as transforming governing partial differential equations (PDEs), which are said to be in the strong form, to the weak form where they are readily discretized [18]. Here an Euler-Lagrange approach stemming from variational calculus is used to derive the governing PDE, which is subsequently discretized.
First, the Lagrangian is derived for a mechanical system considering only conservative energies. The Lagrangian is defined as the difference between kinetic and potential energy, equation 4.1, [151]. As was discussed in chapter 3, the conservative volumetric potential energy is given by the shaded region highlighting the linear-elastic regime of the stress-strain curve in figure 4.1. Hence the total potential energy is described mathematically by equation 4.2. The kinetic energy is given by equation 4.3, and is dependent on the system’s momentum, $\dot{\psi}$.

$$L = T^{total} - U^{total} \quad (4.1)$$

$$U = \int_{V} \frac{1}{2} \sigma \epsilon dV \quad (4.2)$$

$$T = \int_{V} \frac{1}{2} \rho \dot{\psi}^2 dV \quad (4.3)$$

It follows from equations 4.2 and 4.3 that the Lagrangian is of the form,

$$L(\psi, \dot{\psi}) \quad (4.4)$$

In the field of variational calculus it was shown by Euler that for equations of this form, solutions to equation 4.5 minimize equation 4.6, [151]. Equation 4.5 is called the Euler-lagrange equation of motion, and for the described Lagrangian it is the governing equation of motion for a mechanical domain.

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{u}_k} \right) - \frac{\partial L}{\partial u_k} = F_k \quad (4.5)$$

$$\delta \int_{t_1}^{t_2} L dt = 0 \quad (4.6)$$

Next, the energy terms need to be discretized so that the FEM formulation of equation 4.5 can be constructed. Discretization is achieved by use of shape functions. Shape
functions are interpolating functions used to approximate quantities of interest at locations not corresponding to nodal points. Shape functions are thoroughly described in any FEM or BEM book and thus will not be described further here. For more information on this topic the reader is directed to references [146, 18]. The displacement field is discretized by some set of shape functions, $N$, which are independent of time, equation 4.7.

$$\psi = Nu$$  \hspace{1cm} (4.7)

Because the shape functions are independent of time the first derivative of $\psi$ with respect to time – velocity – is interpolated by the same shape functions used to approximate displacement, equation 4.8. Therefore, the kinetic energy is discretized using some adequate set of shape functions $N$ by substituting equation 4.8 into equation 4.3, which leads to
equation 4.9.

\[ \dot{\psi} = N \dot{u} \] (4.8)

\[ T_{el} = \int_V \frac{1}{2} \rho \ddot{u}_{el}^T N^T N \dot{u}_{el} dV \] (4.9)

From equation 4.9 the elemental mass matrix is defined by equation 6.3. By substituting this definition back into equation 4.9 we can write the elemental kinetic energy in a more compact and recognizable form, equation 4.11.

\[ M_{el} = \int_V \rho N^T N dV \] (4.10)

\[ T_{el} = \frac{1}{2} \ddot{u}_{el}^T M_{el} \dot{u}_{el} \] (4.11)

The potential energy can be discretized by similar considerations. The potential energy is calculated via the contraction of the stress and strain tensors. Strain is computed via partials of the displacement field with respect to space. In 2-dimensions strain is given by equation 4.12, a similar but slightly more complex equation represents the 3-dimensional stress tensor. Now, the shape functions may be time invariant, but they are dependent on space, thus the computation of the strain using a discretized displacement field leads to equation 4.13. Here the strain field is interpolated by the differential operator \( B \), which is a non-square matrix composed of partials of \( N \), [146, 18].

\[ \epsilon = \begin{bmatrix} \frac{\partial \psi}{\partial x} \\ \frac{\partial \psi}{\partial y} \\ \frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} \end{bmatrix} \] (4.12)

\[ \epsilon = Bu \] (4.13)
In mechanics stress and strain are related by constitutive models which are functions of specific material properties. A discretized constitutive relationship between stress and strain for a homogenous, linear isotropic material is given equation 4.14, [146, 18].

\[ \sigma = D \epsilon \]

\[ \Rightarrow \sigma = DBu \] (4.14)

Therefore, by applying the constitutive equation to equation 4.2, the elemental potential energy can be written in terms of displacement, the differential operator, and the constitutive matrix, equation 4.15. The elemental stiffness matrix is defined in equation 4.16, and therefore the elemental potential energy can be compactly expressed by equation 4.17.

\[ U_{el} = \frac{1}{2} u_{el}^T B^T DBu_{el} dV \] (4.15)

\[ K_{el} = \int_V \frac{1}{2} B^T D B dV \] (4.16)

\[ U_{el} = \frac{1}{2} u_{el}^T K_{el} u_{el} \] (4.17)

Finally, substituting the expressions for discretized elemental potential and kinetic energies, equations 4.11 and 4.17, into the Euler-Lagrange equation of motion, equation 4.5, we arrive at the discretized equation of motion for the mechanical system, equation 4.18.

\[ L = T - U \]

\[ \Rightarrow L = \frac{1}{2} \dot{u}^T M \ddot{u} - \frac{1}{2} u^T K u \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{u}_k} \right) - \frac{\partial L}{\partial u_k} = F_k \]

\[ \Rightarrow \frac{d}{dt} \left( \frac{1}{2} \dot{u}^T M \ddot{u} - \frac{1}{2} u^T K u \right) - \frac{\partial}{\partial u} \left( \frac{1}{2} \dot{u}^T M \ddot{u} - \frac{1}{2} u^T K u \right) = f_{applied} \] (4.18)

\[ \Rightarrow \frac{d}{dt} (M \ddot{u}) + Ku = f_{applied} \]

\[ \Rightarrow M \ddot{u} + Ku = f_{applied} \]
The equation of motion developed here is general, in that it is equally applicable for 1, 2 or 3-dimensional problems. To complete the model one needs simply to pick shape functions/elements and constitutive laws appropriate to the dimensionality/complexity of the intended problem. The software developed in this chapter, and given by appendix F, is a 2-dimensional model, and uses linear plane stress elements and associated constitutive laws to approximate the mechanical domain. More information about these specific elements and constitutive laws can be found in [146, 18].

The computational model developed by this research investigates mechanical loading by electrostatic forces only. The calculation of these forces is rather simple, but requires knowledge of the electric field at the boundary of the mechanical and electric domains. The derivation of the electric field solver developed for this purpose is focus of the next 2 sections.

4.4 Formulation of the Faux-Lagrangian Finite Difference Solver for application to Electrostatics/Potential Problems

In the preceding section the equation of motion for the mechanical domain of the multi-physics model was derived using an Euler-Lagrange formulation. At this point we know the PDE governing the motion of a mechanical system subjected to some load, but as of yet, we do not know how to calculate that load. Specifically, the systems considered by this work are electrostatically actuated MEMS and NEMS switches having aspect ratios $< 10^{-2}$. Thus the loads applied to the mechanical solution are electrostatic forces which result from charge distributions. In the following two sections modeling of the electrostatic-domain and the derivation of a faux-Lagrangian finite-difference solver for potential problems will be discussed in detail.

4.4.1 Governing Equations

Maxwell’s equations are a set of partial differential equations (PDEs) that describe how the electric and magnetic, $\mathbf{B}$, fields relate to their sources, namely, charge density, $\rho$, 

...
and current density, \( J \). These equations are the foundation of classical electrodynamics. A good introduction to electrodynamics is Griffith’s book aptly titled, "Introduction to Electrodynamics." In their differential form, Maxwell’s equations are given by,

\[
\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \quad (4.19)
\]

\[
\nabla \cdot \mathbf{B} = 0 \quad (4.20)
\]

\[
\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (4.21)
\]

\[
\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \quad (4.22)
\]

The electrostatic force can be derived from the Lorentz Force Law [80] and is given by the simple expression,

\[
F_{\text{elect.}} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (4.23)
\]

For the model developed here we will assume that the system is quasi-static, that there are no magnetic materials, and that there are no bound charges. Thus to solve for the E-field we only need to consider the first and third equation in the set of Maxwell’s equations given above. In electrodynamics these equations are known as Gauss’ Law, (mathematically it is Poisson’s equation), and Faraday’s law. From our assumptions these equations reduce to,

\[
\nabla \cdot \mathbf{E} = 0 \quad (4.24)
\]

\[
\nabla \times \mathbf{E} = 0 \quad (4.25)
\]

For our stated assumptions the Lorentz force law reduces to,

\[
F_{\text{elect}} = q\mathbf{E} \quad (4.26)
\]

Therefore, to calculate the electrostatic load we will need to calculate the charge distribution, \( q \), at the boundary of the mechanical domain, and the the electric field, \( \mathbf{E} \), between
the deformable source and fixed actuating electrode/s. The charge distribution is easily approximated, so we will first turn our attention to the E-field.

Now, any vector field whose curl is 0 can be given by gradient of a scalar potential [128], and via application of Stoke’s equation it can be shown for our assumptions that the electric field is the negative of the gradient of a scalar potential, called the electric potential, equation 4.27.

\[ \mathbf{E} = -\nabla \Phi \] (4.27)

Substituting this equation into Gauss’ Law, equation 4.24, we have,

\[ \nabla \cdot (\nabla \Phi) = 0 \] (4.28)

which is by definition Laplace’s equation, 4.29

\[ \Delta \Phi = 0 \] (4.29)

Here the symbol \( \Delta \) is the Laplacian operator, for 2-D Cartesian coordinates defined as,

\[ \Delta (\bullet) = \frac{\partial^2}{\partial x^2} (\bullet) + \frac{\partial^2}{\partial y^2} (\bullet) \] (4.30)

Therefore we can calculate the electric field by first solving the much easier scalar potential Laplace’s equation.

4.4.2 The Faux-Lagrangian Finite Difference Scheme

The electrostatic domain will be represented by a faux-Lagrangian (FL) mesh. In this way, field points in the mesh can be generated and easily tracked through out the analysis. Typically the potential problem is solved using the BEM method, which becomes increasingly difficult and requires specialized integration schemes for low aspect ratio domains [15]. Here
Laplace’s equation will be solved using a novel finite difference based scheme adaptive to quasi-statically deforming domains.

The nodal points of the FL electrostatic mesh are used for nothing more than their coordinates in Cartesian and Row-Column space. In the method presented, information about each node, i.e., it’s Cartesian coordinates, nearest neighbor distance, electric potential, and eventually electric field, are stored as an element in a matrix. A node’s information is mapped to various matrices via a one-to-one transformation based on the the node’s location in the FL mesh, figure 4.2. In this way a finite-element construction can be used to aid in the solution of a finite difference problem. The utility of this method will become apparent when considering the coupled domain deformation of the electrostatic and mechanical domains.

![Figure 4.2: Mapping of the FL mesh to some matrix A; nodal information for some node k of the FL mesh is mapped to its geometrically equivalent location in a the equivalent A, via homeomorphic transformation T](image)

### 4.4.2.1 1\textsuperscript{st} and 2\textsuperscript{nd} Order Finite Difference Methods

The electrostatic domain is represented by a 2-D model. Because domain is 2-D, it is finite and bounded. Because the domain is bounded, the solution of Laplace’s equation will require the use of 3 different finite difference schemes: backward, forward and central. The 1\textsuperscript{st} order schemes for a continuous function are derived from the fundamental definition of a derivative, and given by equation set 4.33.
The 2nd order schemes are derived by application of the definition of the derivative to the 1st order schemes.

\[
\begin{align*}
    f'(x)_B & \approx \frac{f(x) - f(x - \Delta x)}{\Delta x} \\
    f'(x)_F & \approx \frac{f(x + \Delta x) - f(x)}{\Delta x} \\
    f'(x)_C & \approx \frac{f(x + \Delta x/2) - f(x - \Delta x/2)}{\Delta x}
\end{align*}
\]

Because only a discrete number of points in the electrostatic domain are considered, the finite difference schemes need to be modified. The discretized forms of these equations are given by equations 4.33 and 4.34.

\[
\begin{align*}
    f''(x)_B & \approx \frac{f(x) - 2f(x - \Delta x) + f(x - 2\Delta x)}{\Delta x^2} \\
    f''(x)_F & \approx \frac{f(x + 2\Delta x) - 2f(x + \Delta x) + f(x)}{\Delta x^2} \\
    f''(x)_C & \approx \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2}
\end{align*}
\]

Extending the discretized 2nd order schemes to 2-D and substituting them into equation 4.29, we have the following three different finite difference representations for Laplace’s equation.

\[
\begin{align*}
    f'_i & \approx \frac{f_{i+1} - f_i}{\Delta x} \\
    f'_F & \approx \frac{f_{i+1} - f_i}{\Delta x} \\
    f'_C & \approx \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} \\
    f''_B & \approx \frac{f_{i-2} - 2f_{i-1} + f_i}{\Delta x^2} \\
    f''_F & \approx \frac{f_{i+2} - 2f_{i+1} + f_i}{\Delta x^2} \\
    f''_C & \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}
\end{align*}
\]

4.4.2.2 The backward difference formulation

\[
\Delta \Phi_{(i,j)B} = \frac{\Phi_{(i,j)} - 2\Phi_{(i,j-1)} + \Phi_{(i,j-2)}}{\Delta x^2} + \frac{\Phi_{(i,j)} - 2\Phi_{(i-1,j)} + \Phi_{(i-2,j)}}{\Delta y^2} = 0
\]
4.4.2.3 The forward difference formulation

\[
\Delta \Phi_{(i,j)} = \frac{\Phi_{(i,j+2)} - 2\Phi_{(i,j+1)} + \Phi_{(i,j)}}{\Delta x^2} + \frac{\Phi_{(i+2,j)} - 2\Phi_{(i+1,j)} + \Phi_{(i,j)}}{\Delta y^2} = 0
\]  

(4.36)

4.4.2.4 The central difference formulation

\[
\Delta \Phi_{(i,j)C} = \frac{\Phi_{(i,j+1)} - 2\Phi_{(i,j)} + \Phi_{(i,j-1)}}{\Delta x^2} + \frac{\Phi_{(i+1,j)} - 2\Phi_{(i,j)} + \Phi_{(i-1,j)}}{\Delta y^2} = 0
\]  

(4.37)

In the case of an undeformed, and/or ungraduated-mesh, as shown in figure 4.3, the spacing between nearest neighbors is equal in x and y, equation 4.41.

![Figure 4.3: FL nodal Nearest neighbor distances for an undeformed mesh](image)

\[
\Delta x_{(i,j)F} = \Delta x_{(i,j)B} = \Delta x_{(i,j)} \\
\Delta y_{(i,j)F} = \Delta y_{(i,j)B} = \Delta y_{(i,j)}
\]  

(4.38)

However, for a deformed/graduated mesh, as shown in figure 4.4, the spacing between nearest neighbors is not generally equal in the x or y directions, equation 4.39.
To overcome this, we replace $\Delta x$ and $\Delta y$ in equations 4.35-4.37, with average radial distances between nearest neighbors in the finite-difference mesh, equation 4.40.

$$\Delta \tilde{r}_x = \frac{\Delta r_{x,B} + \Delta r_{x,F}}{2}$$

$$\Delta \tilde{r}_y = \frac{\Delta r_{y,B} + \Delta r_{y,F}}{2}$$  (4.40)

The definitions of $\Delta r_{xB}$, $\Delta r_{xF}$, $\Delta r_{yB}$, and $\Delta r_{yF}$ for an interior node (a node with coordination number 4), are given below, and illustrated in figure 4.5. From these definitions the average-radial distance for boundary nodes and corner nodes follows, equations 4.42-4.45 for boundary nodes, and equations 4.46-4.49, illustrated in figure 4.6.
Figure 4.5: FL nodal nearest neighbors in terms of forward and backward radii

\[ \Delta r_x^{(i,j)} = \sqrt{(x_{(i,j-1)} - x_{(i,j)})^2 + (y_{(i,j-1)} - y_{(i,j)})^2} \]
\[ \Delta r_F^{(i,j)} = \sqrt{(x_{(i,j+1)} - x_{(i,j)})^2 + (y_{(i,j+1)} - y_{(i,j)})^2} \]
\[ \Delta r_y^{(i,j)} = \sqrt{(x_{(i,j-1)} - x_{(i,j)})^2 + (y_{(i,j+1)} - y_{(i,j)})^2} \]
\[ \Delta r_B^{(i,j)} = \sqrt{(x_{(i-1,j)} - x_{(i,j)})^2 + (y_{(i-1,j)} - y_{(i,j)})^2} \]
\[ \Delta r_F^{(i,j)} = \sqrt{(x_{(i+1,j)} - x_{(i,j)})^2 + (y_{(i+1,j)} - y_{(i,j)})^2} \]

(4.41)

**4.4.3 Average Radial Distances for Special Boundaries**

**Boundary Case 1: \( n = \{0, -1\} \)**

\[ \Delta \tilde{r}_x = \frac{\Delta r_x B + \Delta r_x F}{2} \]
\[ \Delta \tilde{r}_y = \Delta r_y F \]

(4.42)

**Boundary Case 2: \( n = \{1, 0\} \)**

\[ \Delta \tilde{r}_x = \Delta r_x F \]
\[ \Delta \tilde{r}_y = \frac{\Delta r_y B + \Delta r_y F}{2} \]

(4.43)
Boundary Case 3: \( n = \{0, 1\} \)

\[
\Delta \tilde{r}_x = \frac{\Delta r_{xB} + \Delta r_{xF}}{2} \\
\Delta \tilde{r}_y = \Delta r_{yB}
\]  

(4.44)

Boundary Case 4: \( n = \{-1, 0\} \)

\[
\Delta \tilde{r}_x = \Delta r_{xB} \\
\Delta \tilde{r}_y = \frac{\Delta r_{yB} + \Delta r_{yF}}{2}
\]

(4.45)

4.4.3.1 Average Radial Distances for Corners

Corner Case 1:

\[
\Delta \tilde{r}_x = \Delta r_{xF} \\
\Delta \tilde{r}_y = \Delta r_{yF}
\]

(4.46)

Corner Case 2:

\[
\Delta \tilde{r}_x = \Delta r_{xF} \\
\Delta \tilde{r}_y = \Delta r_{yB}
\]

(4.47)

Corner Case 3:

\[
\Delta \tilde{r}_x = \Delta r_{xB} \\
\Delta \tilde{r}_y = \Delta r_{yB}
\]

(4.48)

Corner Case 4:

\[
\Delta \tilde{r}_x = \Delta r_{xB} \\
\Delta \tilde{r}_y = \Delta r_{yF}
\]

(4.49)

All of the necessary frame-work has now been developed to solve Laplace’s equation using the developed FL finite-difference scheme for quasi-statically deformed, low aspect-ratio, domains. To complete the derivation of the method, we replace \( \Delta x \) and \( \Delta y \) in equations 4.35-4.37 with the appropriate expressions of \( \Delta \tilde{r}_x \) and \( \Delta \tilde{r}_y \) and solve for \( \Phi_{(i,j)} \), equation 4.50.

\[
\frac{\Phi_{(i,j+1)} - 2\Phi_{(i,j)} + \Phi_{(i,j-1)}}{\Delta \tilde{r}_{(i,j)}^2} + \frac{\Phi_{(i+1,j)} - 2\Phi_{(i,j)} + \Phi_{(i-1,j)}}{\Delta \tilde{r}_{(i,j)}^2} = 0
\]

\[
\Rightarrow \frac{1}{2(\Delta \tilde{r}_{(i,j)}^2 + \Delta \tilde{r}_{(i,j)}^2)} \left[ \Delta \tilde{r}_{(i,j)}^2 (\Phi_{(i,j+1)} + \Phi_{(i,j-1)}) + \Delta \tilde{r}_{(i,j)}^2 (\Phi_{(i+1,j)} + \Phi_{(i-1,j)}) \right] = \Phi_{(i,j)}
\]

(4.50)
4.4.4 Application of Boundary Conditions

There are two possible boundary conditions for Laplace’s equation, namely, Dirchlet and Neumann boundary conditions. A Dirchlet BC means that a potential is prescribed on a boundary. The application of these conditions is the most simple and requires only that boundary nodes be set equivalent to the prescribed potential. The second kind of condition, the Neumann BC, means that the constraint is in regard to the flux through a boundary. The devices developed in chapter 5 are fabricated in such a way that some of boundary edges of the electrostatic domain are dielectrics, which implies that no potential can be applied to those boundaries. The Neumann BC applied to these oxide boundaries is most simply stated by equation 4.51. The BC states that the flux-normal to the boundary is exactly 0. For the electric potential this means that there is no electric field normal to an oxide boundary. A simple rectangular electrostatic domain is illustrated in figure 4.7. The figure shows two conducting boundaries with a potential applied across them, depicted by illustrating the resulting charge accumulation (Dirchlet), and two oxide boundaries with the Neumann boundary condition described by equation 4.51.
\[ \frac{\partial \Phi}{\partial n} = \nabla \Phi \cdot \mathbf{n} = 0 \quad (4.51) \]

Figure 4.7: Illustration of a simple rectangular electrostatic domain with Robin boundary conditions

The fabrication processes developed by this research results in devices whose electrostatic domains can be approximated best by rectangular shapes. This means that the boundaries will always be parallel to either the x- or y cartesian coordinate frame, thus the Neumann BC can be directly applied to Laplace’s equation, resulting in equations 4.53 and 4.54, the solutions to Laplace’s equation on electrostatic domain boundaries adjacent to dielectrics.

### 4.4.5 Solutions to Laplace’s Equation on Dielectric Boundaries

For dielectric boundaries described by \( \mathbf{n} = \pm 1, 0 \), equation 4.51 is,

\[ \nabla \Phi \cdot \mathbf{n} = \left\{ \frac{\partial \Phi}{\partial x}, \frac{\partial \Phi}{\partial y} \right\} \cdot \{ \pm 1, 0 \} = 0 \]

thus,

\[ \frac{\partial \Phi}{\partial x} = \frac{\partial^2 \Phi}{\partial x^2} = 0 \quad (4.52) \]

It follows that application of the Neumann BC to 4.37 yields the solution to Laplace’s equation on such boundaries, equation 4.53.
\[
\Delta \Phi_{(i,j)} = \frac{\partial \Phi_{i,j}}{\partial x} = \frac{\Phi_{(i+1,j)} - 2\Phi_{(i,j)} + \Phi_{(i-1,j)}}{\Delta r_{(i,j)}^2} = 0
\]

\[
\Rightarrow \frac{1}{2} \left( \Phi_{(i+1,j)} + \Phi_{(i-1,j)} \right) = \Phi_{(i,j)}
\]

Vs. to boundaries described by \( \mathbf{n} = \{0, \pm 1\} \) yields the following solution to Laplace’s equation on those boundaries,

\[
\Delta \Phi_{(i,j)} = \frac{\partial \Phi_{i,j}}{\partial x} = \frac{\Phi_{(i,j+1)} - 2\Phi_{(i,j)} + \Phi_{(i,j-1)}}{\Delta r_{(i,j)}^2} = 0
\]

\[
\Rightarrow \frac{1}{2} \left( \Phi_{(i,j+1)} + \Phi_{(i,j-1)} \right) = \Phi_{(i,j)}
\]

The preceding derivation allows us to solve Laplace’s equation in deformable, low-aspect ratio electrostatic domains. Following an initial guess of the potential field, the solver is iterated until convergence criteria are satisfied. Once the Electric potential at each node is known, the electric field at each node can be quickly calculated using equation 4.27. This can be accomplished using the 1\(^{st}\) order finite difference schemes derived above, equation 4.33. Care needs to be taken to ensure that the proper scheme, i.e. backward, forward or central, is used. The gradient method is not discussed in detail, but MatLab code for it’s implementation is provided in Appendix F.

### 4.5 Calculation of Electrostatic Loads

Once the electric field has been calculated for each nodal point, the electrostatic force applied to the mechanical domain is calculated using equation 4.55, which is the discretized form of the simplified Lorentz force law. To calculate the nodal charge distribution, \( q_j \), required for the calculation, each element of the mechanical domain, corresponding to the mechanical/electric domain interface, is approximated to be a parallel plate capacitor, and the elemental charge first computed.

\[
F_j = q_j E_j
\]

The elemental charge is approximated by equation 4.56, and the capacitance by equa-
tion 4.57. Because the devices considered by this FEM model have $g:L$ ratios on the order of $10^{-3}$, the ratio of displacement to length prior to snap-thru is of the same order. For this reason very little curvature is experienced by the beam prior to snap through, which implies that each element experiences negligible rotation, and the use of a parallel plate approximation is justified. In figure 4.8 a diagram illustrating parallel plate capacitance discretization parameter definitions is given. Elemental indices are indexed by $i$, and nodal indices are indexed by $j$.

$$q_{el}^i = C_{el}^i V$$  \hspace{1cm} (4.56)$$

$$C_{el}^i = \frac{\varepsilon_o A^i}{g_o - \bar{u}^i}$$  \hspace{1cm} (4.57)$$

Here $\bar{u}^i$ is the average elemental displacement calculated by,

$$\bar{u}^i = \frac{u_{j+1} + u_j}{2}$$  \hspace{1cm} (4.58)$$

therefore the elemental capacitance is more explicitly given by,

$$C_{el}^i = \frac{2\varepsilon_o A^i}{2g_o - (u_{j+1} + u_j)}$$  \hspace{1cm} (4.59)$$

The total capacitance of the device is calculated by approximating the structure as being composed of elemental capacitors in parallel. Thus, the total capacitance is simply the sum of elemental capacitances, equation 4.60. In the equation $N$ is the total number of elements used to approximate the capacitor surface.

$$C_{total} = \sum_{i=1}^{N} C_{el}^i$$  \hspace{1cm} (4.60)$$

Once the the elemental capacitance has been calculated, for element $i$, the elemental charge is calculated using equation 4.56 and then distributed to the elemental nodes via equation 4.61. In this way the elemental charge is distributed to the mesh nodes. In FEM
and BEM, this is a standard practice; scalar values are calculated at elemental centers, and vector quantities are calculated at elemental nodes.

\[ q_j = \frac{q_{ele}^j + q_{ele}^{j-1}}{2} \]  \hspace{1cm} (4.61)

Finally, the electrostatic force at each node of the mechanical domain is calculated using equation 4.55. The process is repeated for each element of the mechanical corresponding to the mechanical/electric domain interface to construct the total surface load vector \( F_{elect} \). The surface load vector is then passed to the mechanical solver where the nodal displacements, velocities, and accelerations of the mechanical domain are updated/calculated.

### 4.6 Non-linear (NL) Integration scheme

Because of the applied electrostatic load, the discretized equation of motion describing the system dynamics is non-linear. Therefore, to solve the NL equation of motion, equation 4.18, a non-linear time integration scheme is required. For this task the NL Newmark scheme has been chosen and implemented in the developed software, appendix F. The scheme is implicit-explicit, which means that time integration is accomplished using predicted information about future system quantities, i.e, displacement, velocity and acceleration, as

---

**Figure 4.8:** Diagram illustrating parallel plate capacitance discretization parameter definitions; elemental indices are indexed by \( i \), and nodal indices are indexed by \( j \).
well as known information from the previous time step. The two key components of the scheme are briefly described by the following two sections.

4.6.1 Newmark’s $\beta$ Equations: Implicit-Explicit Time integration

The Newmark $\beta$ equations, as they are called, were first introduced in 1978 by Hughes and Liu [96]. The method is an implicit-explicit scheme based on predictor and corrector equations for displacement, velocity and acceleration of a mechanical system, equations 4.62-4.63. The given system of equations, composed of the set of predictors and correctors, is indeterminate, because there are five unknowns, but only four equations. Therefore, to solve the system of equations, a fifth equation which relates the acceleration to the difference between the corrected displacement and the predicted displacement is introduced, equation 4.64.

predictors:

$$\tilde{u}^{n+1} = u^n + \Delta t v^n + \Delta t^2 (1/2 - \beta) a^n$$

$$\tilde{v}^{n+1} = v^n + \Delta t (1 - \gamma) a^n$$

(4.62)

correctors:

$$u^{n+1} = \tilde{u}^{n+1} + \beta \Delta t^2 a^n$$

$$v^{n+1} = \tilde{v}^{n+1} + \gamma \Delta t a^n$$

(4.63)

$$a^{n+1} = \frac{1}{\beta \Delta t^2} (u^{n+1} - \tilde{u}^{n+1})$$

(4.64)

The given predictor/corrector equations are functions of the parameters $\gamma$ and $\beta$. A physical analogy for the parameter $\gamma$ is given in Belytschko’s book on the NL FEM [18]. Gamma can be thought of as artificial viscosity. This implies that, depending on the value chosen for $\gamma$, a degree of “damping” can be introduced into the integration scheme. Just as an over damped mechanical system tends to quickly kill oscillations, this numerical “damping” parameter can be used to suppress noise in the solution. It should be noted that for $\gamma = 1/2$ no damping is added to the integration scheme. The parameter $\beta$ acts as a shift/switch,
or better yet, a weighting parameter between different integration schemes. For example, a value of 0 results in the explicit central difference method being used for the integration scheme, but a value of $1/4$ shifts the integration scheme to the trapezoidal rule.

It has been reported that the Newmark method is unconditionally stable for $1/4 \leq \gamma/2 \leq \beta$ C.8. Therefore, for all numerical simulations conducted in this research I have chosen to set the integrations parameter as follows: $\beta = 1/4$ and $\gamma$. This implies that the integration scheme employed is undamped, unconditionally stable, and shifted to the the trapezoidal rule. If desired, the integration scheme used by the developed software can be easily changed because the parameters $\gamma$ and $\beta$ are programmed as input options in the MATLAB m-file *MultiPhysicsFEM_V1.m*, which is the first routine given in appendix F.

### 4.6.2 NL Newmark Integration Scheme: Newton’s Method with Newmark’s $\beta$ equations

In order to construct the scheme we first apply equation 4.64 to system residual given by equation 4.65, where $s_D = 0/1$ depending on whether the modeled system is dynamic or static. Initial conditions must be chosen at $t = t_o$, and for most simulations the following initial conditions are appropriate: $u_o = \tilde{u}^{n+1}$ and $u_o^{n+1} = 0$.

$$R = 0 = \frac{s_D}{\beta \Delta t^2} M \left( u^{n+1} - \tilde{u}^{n+1} \right) + \dot{f}_{int} - \dot{f}_{ext} \quad (4.65)$$

To implement the integration scheme the effective tangential stiffness matrix must be calculated. In literature the effective tangential stiffness matrix is sometimes referred to as the system Jacobian matrix. The effective tangential stiffness matrix is derived via a Taylor series expansion of the residual $R$ about some point $u_k$, equation set 4.66. A graphical interpretation of the tangential stiffness matrix and it’s role in Newton’s method illustrated in figure 4.9. In the illustration we see that the matrix is aptly named as it is tangent to the system residual.
\[ R(u_k) + \frac{\partial R(u_k)}{\partial u} \Delta u = 0 \]
\[ \Rightarrow R(u_k) + K_T \Delta u = 0 \]
\[ u = u^{n+1} - \bar{u}^{n+1} \]
\[ \Delta u = u_{k+1} - u_k \] (4.66)

It follows from equation 4.66 that the tangential stiffness matrix of the system is calculated by taking the first partial of the system residual with respect to displacement, equation 4.67. With equation 4.65 we can easily solve for \(\Delta u\), which is the parameter needed to calculate updated displacements, velocities, and accelerations.

\[ K_T = \frac{\partial}{\partial u} \left( \frac{s_D}{\beta \Delta t^2} Mu + f_{int} + f_{ext} \right) = \frac{s_D}{\beta \Delta t^2} M + K \Delta u = u_{k+1} - u_k \] (4.67)
\[ \Delta u = -K_T^{-1} R(u_k, t^{n+1}) \] (4.68)
Finally, the formulas used to update displacements, velocities, and accelerations are given by equation set 4.69. The formulas include a relaxation parameter $\Theta_{NM}$, where $0 < \Theta_{NM} \leq 1$. For implementation of the developed multi-physics model a value of $\Theta_{NM} = 0.85 - 1$ was chosen, which is consistent with reported relaxation parameters used in electrostatic simulations.

\[
\begin{align*}
    u^{n+1} &= d^n + \Theta_{NM} u \\
    v^{n+1} &= v^n + \frac{\gamma}{\beta \Delta t} \Theta_{NM} u \\
    a^{n+1} &= a^n + \frac{\gamma}{\beta \Delta t^2} \Theta_{NM} u
\end{align*}
\]  

(4.69) (4.70) (4.71)

4.7 Verification of Developed FEM Model: Test Cases/Results

The developed model has been validated by comparing the numerically and analytically computed solutions of several different test cases of increasing complexity. Specifically, nodal electric field values calculated using the faux-Lagrange finite difference (FLFD) method are compared to analytically calculated electric fields values. After the accuracy of FLFD electric field solver was verified, the switching behavior of several theoretical WALD NEMS switches were simulated. From these simulations, the fully-coupled electromechanical model has been validated by comparing the FEM calculated pull-in voltages of a 2-terminal WALD switch, 3-terminal WLD switch, and 3-terminal WALD bow-tie switch to pull-in voltages calculated using the analytic model developed in chapter 3 sections 3.2-3.3. Finally, detachment curves have been generated using a van der Waals force module and compared to those derived analytically in chapter 3 section 3.4.3.

4.7.1 Verification of The Electric Field

The numerical electric field solver was first verified by modeling a 2-terminal parallel plate capacitor. This case is the most simple and was used as a check of the software before the FLFD code was extended for 3-terminal capabilities. The device modeled has the
dimensions: \( L = 1 \text{ um} \), and \( g = 1 \text{ um} \). A potential of 10 V was applied between the plates. Results of the simulation are shown in figure 4.10, and summarized in table 4.1.

![2-Terminal Electric Domain: \( V_{GS} = 10 \text{ V} \)](image)

Figure 4.10: 2-Terminal FEM Electrostatic Solution: Electric field magnitude normal to the drain and source is 10 V/um

The 3-terminal FLFD solver was validated by modeling a 3-terminal device for two different cases. The first case considers only a potential applied between the gate and source. Theoretically it is expected that the electric field between the gate and source should be equal to \( V/g_{GS} \). For this gate-actuated case \( V_{GS} = 0.3 \text{ V} \). For the second case, a voltage was applied to both the drain and source boundary while the gate boundary was grounded. In order make the results more interesting, and to validate the FLFD scheme using a more complicated biasing case, 0.3 volts were applied to both the drain and source boundaries. For this case the potential between the drain and source should be 0 V, therefore if the model works no electric field should be calculated in this region. For both models the following dimensions were used: \( L = 4 \text{ um} \), \( D_W = 0.25 \text{ um} \), \( G_W = 1.875 \text{ um} \), \( g_{DS} = 20 \text{ nm} \), and \( g_{GS} = 50 \text{ nm} \). Simulation results are shown in figures 4.11 and 4.12, and summarized in table 4.1.
Figure 4.11: 3-Terminal FEM Electrostatic Solution: Electric field magnitude normal to the gate and source is 6 V/um

Figure 4.12: 3-Terminal FEM electrostatic solution with $V_{DD} = V_{DS}$: Electric field magnitude between gate and drain is $\approx 0$ V/um, which agrees with theory because $\Delta V_{DS} = V_{DS} - V_{DD} = 0$ V

4.7.1.1 Electric field Simulation Results

Table 4.1 lists and compares the results from the electric field simulations to theoretically expected results for the electric field between undeformed parallel plates. For all cases the FLFD results are identical to electric fields calculated analytically using equation 4.72. In the table FLFD calculated electric fields are listed as vectors, and the analytically
calculated electric fields as scalars. This is because the simple 1-D analytic equation given assumes the transverse component of the electric field to be zero. Furthermore, the analytic equation only gives the magnitude of the field in the direction normal to the plates, not it’s direction. Theoretically the electric field flows from negative charges to positive charges, which is seen to be true for all of the numerical simulations.

\[ E = \frac{V}{g} \]  

(4.72)

<table>
<thead>
<tr>
<th>Test Case</th>
<th>FLFD [V/um]</th>
<th>Analytic [V/um]</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-terminal</td>
<td>[0, -10]</td>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>3-terminal, ( V_{GS} = 0.3 ) V</td>
<td>[0, -6]</td>
<td>6</td>
<td>0</td>
</tr>
<tr>
<td>3-terminal ( V_D = V_{DD} = 0.3 ) V</td>
<td>( [4.59 \times 10^{-8}, -1.38 \times 10^{-14}] )</td>
<td>0</td>
<td>( \approx 0 )</td>
</tr>
</tbody>
</table>

4.7.2 Pull-in of Thin-film Electrostatically Actuated Fixed-fixed NEMS Switches with \( g : l \) on the order of \( 10^{-3} \)

In the following simulations all modeled device dimensions were chosen to correspond to length scales feasibly fabricated using the WALD fabrication processes developed by this research effort, and described in chapter 5. For all simulations the material properties of bulk tungsten have been used. Furthermore, because the magnitude of thin-film stress (through-gradient and tensile) in fabricated WALD devices is unknown, the following simulations assume a zero initial stress state in the mechanical domain.

4.7.2.1 A 2-terminal Fixed-Fixed WALD NEMS Switch

For the first test case the switching behavior of a 2-terminal fixed-fixed WALD switch was simulated. Just as for the verification of the FLFD electric field solver, a 2-terminal
device represents the most simple and comparable test case. The dimensions of the simulated 2-terminal device are: 4,000 x 500 x 32 nm (S), $g_{GS} = 50$ nm. The displacement versus applied voltage curve generated by the software is shown in figure 4.13, and results summarized in table 4.2.

4.7.2.2 A 3-terminal Fixed-Fixed WALD NEMS Switch

Next, the switching behavior of a 3-terminal fixed-fixed WALD switch with constant width was simulated. Two simulations corresponding to gate actuation, and drain actuation were conducted. Compared to the 2-terminal case, this case is a significant leap in device, as well as in simulation, complexity. The dimensions of the simulated 2-terminal device are: 4,000 x 500 x 32 nm (S), $D_W = 250$ nm, $G_W = 1.875$ um (x2), $g_{DS} = 20$ nm, and $g_{GS} = 50$ nm. The displacement versus applied voltage curves generated by the software for drain and gate actuation are shown in figures 4.14 and 4.15; results are summarized in table 4.2.

4.7.2.3 A 3-terminal Fixed-Fixed WALD NEMS Bow-tie Switch

For the last test case the switching behavior of a 3-terminal fixed-fixed WALD bow-tie switch was simulated. As before the pull-in behavior of the device was simulated for both drain and gate actuation scenarios. This model is the most complicated test case that can be compared to analytic results. The dimensions of the simulated 2-terminal device are: $L = 4,000$ nm, $W_M = 3.5$ um, $W_o = 0.25$ nm, $t = 32$ nm, $D_W = 250$ nm, $G_W = 1.875$ um (x2), $g_{DS} = 20$ nm, and $g_{GS} = 50$ nm. The displacement versus applied voltage curves generated by the software for drain and gate actuation are shown in figures 4.16 and 4.17; results are summarized in table 4.2.

4.7.2.4 Electromechanically Actuated WALD NEMS Simulation Results

There is a large disparity between FEM and analytically calculated pull-in voltages. For all cases considered the pull-in voltages calculated using the developed numerical model
Table 4.2: Comparison of FEM and Analytically Calculated Pull-in Voltages

<table>
<thead>
<tr>
<th>Case</th>
<th>FEM [V]</th>
<th>Analytic [V]</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-terminal</td>
<td>1.68</td>
<td>1.22</td>
<td>37</td>
</tr>
<tr>
<td>3-terminal constant width (D)</td>
<td>2.88</td>
<td>1.88</td>
<td>53</td>
</tr>
<tr>
<td>3-terminal constant width (G)</td>
<td>3.24</td>
<td>2.8</td>
<td>15</td>
</tr>
<tr>
<td>3-terminal bow-tie (D)</td>
<td>2.9</td>
<td>1.86</td>
<td>55</td>
</tr>
<tr>
<td>3-terminal bow-tie (G)</td>
<td>1.48</td>
<td>1.83</td>
<td>19</td>
</tr>
</tbody>
</table>

Table 4.3: FEM and Analytically Calculated Critical Displacements

<table>
<thead>
<tr>
<th>Case</th>
<th>FEM [nm / g&lt;sub&gt;cr&lt;/sub&gt;/g&lt;sub&gt;o&lt;/sub&gt;]</th>
<th>Analytic [nm / g&lt;sub&gt;cr&lt;/sub&gt;/g&lt;sub&gt;o&lt;/sub&gt;]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-terminal</td>
<td>11.6/ 38.7</td>
<td>10/ 33.3</td>
</tr>
<tr>
<td>3-terminal constant width (D)</td>
<td>8.1/ 40.5</td>
<td>6.667/ 33.3</td>
</tr>
<tr>
<td>3-terminal constant width (G)</td>
<td>21.8/ 43.6</td>
<td>16.667/ 33.3</td>
</tr>
<tr>
<td>3-terminal bow-tie (D)</td>
<td>8.6/ 43.0</td>
<td>6.667/ 33.3</td>
</tr>
<tr>
<td>3-terminal bow-tie (G)</td>
<td>21.8/ 43.6</td>
<td>16.667/ 33.3</td>
</tr>
</tbody>
</table>

are larger than those calculated using the 1-D lumped mass analytic models developed in chapter 3, sections 3.2-3.3. The pull-in voltages extracted from each pull-in simulation are listed and compared to corresponding pull-in voltages calculated using the developed analytic models in table 4.2.

For argument’s sake, the displacement at pull-in, g<sub>cr</sub>, and g<sub>cr</sub>/g<sub>o</sub> calculated via FEM and analytic equations for each test case, are listed in table 4.3. It is seen that for the FEM model, which considers charge and associated load distribution, critical displacements are on average 41.2 ± 1.93% of the initial gap height for each geometry considered, while this value is exactly 33.333 % for analytic solutions derived from 1-D lumped mass models. The displacements calculate via FEM agree well with critical displacements calculated from distributed load models, as well as experimentally measured displacements, which have been reported to be anywhere from 40-60 % of the initial gap height. One would therefore expect an increase in pull-in voltage to achieve the increased displacement prior to pull-in.

Finally, the lumped mass model neglects actual structure deformation, thus all elec-
t trostatic loads are applied to a flat plate. In actuality the electrostatically deformed thin film structure results in a non-zero electric field component in the \( i \)-direction, which subsequently reduces the total downward load on the mechanical structure. Because of the symmetric displacement profile of an electrostatically deforming structure, the induced load in the \( i \)-direction places the structure in tension, resulting in some degree of electrostatic stiffening. Furthermore, the pull-in voltages calculated for 3-terminal devices using this model more closely approximate experimentally characterized pull-in voltages for fabricated devices reported in chapter 6. For these reasons although the simulated pull-in voltages are upward of 50% larger than analytically calculated values, the developed model is considered to accurately approximate the switching behavior of thin-film electrostatically actuated devices with functional gap to length ratios on the order of \( 10^{-3} \).

### 4.7.3 FEM Generated Detachment Curves

In chapter 3 section 3.4.3 detachment curves for fixed-fixed and cantilever beams were analytically derived for a system subject to substantial van der Waals interaction. It was shown that the maximum length a beam can have before the van der Waals interaction causes it to collapse and stick to the substrate is linearly dependent on the minimum possible gap height. The equations were derived from a 1-D mass-spring system and are applicable only to MEMS/NEMS devices having rectangular structures of constant width and gap height. To demonstrate the utility of the developed FEM code, the detachment curves have been generated numerically using a specially coded van der Waals force module which is given in appendix G.

The elemental van der Waals loads are calculated from the discretized form of equation C.1, given by 4.73. The variables in equation 4.73 have been previously defined in figure 4.8. Just as with applied electrostatic loads, the elemental van der Waals loads must be distributed to the elemental nodes, and this is accomplished via equation 4.74.
\[ f_{eleVDW}^i = \frac{A_{132}A_{el}^i}{6\pi (2g_o + u_j - u_{j+1})^3} \]  
\[ f_{VDW,j} = \frac{f_{eleVDW}^i + f_{eleVDW}^{i-1}}{2} \]  

Using the van der Waals module detachment curves for a 2-terminal fixed-fixed WALD structure of constant width, and a 2-terminal fixed-fixed WALD bow-tie structure, have been generated. For comparison’s sake, the FEM calculated detachment curves are plotted against the analytically calculated curves for a fixed-fixed and cantilever WALD structure, figure 4.18. The detachment curve for the bow-tie structure was calculated by varying the width of the structure and scaling the bow-tie parameters accordingly. Thus the bow-tie detachment curve shown in figure is specifically for a WALD bow-tie structure having the following proportions: \( W_o = 0.06L \), \( W_M = 0.7L \), and \( D_W = 0.06L \), which are the proportions of the 3-terminal WALD devices fabricated and tested chapters 5 and 6. For all structures considered the thin film thickness was held constant at 32 nm. Finally, all curves were calculated assuming bulk tungsten material properties and zero initial stress, and \( A_{132} = 22 \times 10^{-20} \) J, which was calculated for a W-Au material system using the equations derived in Appendix C.

### 4.7.3.1 FEM Generated Detachment Results

The FEM generated detachment curves in figure 4.18 both have strong linear trends which was expected based on analytic calculations. In the figure we see that the FEM generated detachment curve for the WALD structure having constant width agrees well with the analytic curve. The primary difference between the two curves is that the FEM calculated curve has a steep slope which implies that the critical gap height for any given beam of length \( L \) is somewhat less than predicted analytically, with the difference between approximations becoming larger for increasing length. This is to be expected because the
FEM model considers distributed loads, while the analytic model does not. Because the analytic model is derived from a 1-D ODE, it considers the gap height along the length of the beam to be constant for all applied loads, and therefore overestimates the actual applied load for a given separation distance, which is responsible for the disparity between the two curves.

The detachment length for the bow-ties structure maintains a linear dependence on gap height but has a much smaller slope than either of the curves calculated for fixed-fixed structures of constant width. This is to be expected due to the increased surface area of the bow-tie structure. Because the van der Waals force is linearly proportional to surface area, the force exerted on a bow-tie structure of length $L$ is much greater than that exerted on rectangular structure of the same length. Thus, compared to a rectangular structure, for a bow-tie structure of any length $L$, the critical gap height must be increased in order to attenuate the van der Waals interaction and thereby prevent collapse and stiction.

4.7.3.2 Detachment as a Function of Bow-tie Parameter $W_M$

To further study the effects of van der Waals interaction on WALD bow-tie structures, a study was conducted to investigate the dependence of the critical gap height on the bow-tie parameter $W_M$. The study was conducted by calculating the critical gap height as a function of $W_M$ for various structure lengths. For the study the WALD geometry was again scaled in proportion to the structure length by: $W_o = 0.05L$ and $D_W = 0.06L$, with $t = 32$ nm. Results are plotted in figure 4.19.

For all lengths investigated it is observed that the relationship between critical gap height and $W_M$ is best described by the power law $g(L, W_M) = \alpha(l)W_M^\beta$. The coefficients $\alpha$ and $\beta$ are derived following the same methodological framework described in chapter 3 section 3.5, which was employed to derive the empirical formula for the magnitude of the electric field at a corner. To this end, in figures 4.20a and b, $\alpha$ and $\beta$ have been plotted as functions of $L$. From these plots it was observed that for the investigated bow-tie proportions the coefficient
\( \alpha \) is quadratically dependent on the structure length, and that the power coefficient \( \beta \) is independent of length.

Thus, by fitting \( \alpha \) with a 2\(^{nd} \) order polynomial, and taking \( \beta \) to be the average value of each fit from figure 4.19, an analytic equation for the minimum gap height for a WALD bow-tie structure having the described proportions has been successfully derived from numerical simulations, equation 4.75.

\[
g(L, W_M)_{cr} = (0.199L^2 + 1.1596L + 6.3) W_M^{0.1576} \tag{4.75}
\]

### 4.7.3.3 Bow-tie Detachment Results

Using this analytic equation points have been plotted over the FEM generated bow-tie detachment curve for \( L = 6, 13, 19.4 \) um and \( W_M = 1 : 2 : 11 \) um, figure 4.21. As could be surmised, increasing the bow-tie parameter \( W_M \) for a structure of any given length increases the minimum gap height necessary to prevent stiction, while decreasing \( W_M \) has the opposite effect. As \( W_M \) approaches \( W_o \), the bow-tie detachment curve approaches the detachment curve for a rectangular structure. Finally, for constant \( W_M \) the detachment curve \( L \) versus gap height remains linear, with only the slope effected by choice of \( W_M \).

### 4.7.3.4 Detachment Study Conclusions

The studies reported here are important for several reasons. First, they demonstrate that the van der Waals force module given in appendix G can be used to sufficiently approximate the van der Waals interaction for various MEMS/NEMS devices. Therefore it has also been shown that equation 4.74 is a sufficiently discretized form of equation C.1 which was derived by Lifshitz for continuums, which means that complicated non-linear interactions can be sufficiently described by simple closed form equations. It follows that Casimir forces may also be similarly approximated. Secondly, the empirical derivation of equation 4.75 shows that a library of empirical functions describing the detachment parameters for any structure
having a symmetric profile, e.g. poly-tie structures, may be derived. These equations would significantly reduce time spent on experimental design iterations. Finally, because the generation of detachment curves for 2-terminal (constant gap) devices was proved successful, there is no reason that various detachment curves could not be generated for \( n \)-terminal devices having symmetric profiles, with up to \( n \)-different gap heights.
Figure 4.13: 2-terminal WALD NEMS switch FEM simulation; Model dimensions: 4,000 x 500 x 32 nm (S), and $g_{GS} = 50$ nm; $V_{Pullin} = 1.68$ V

Figure 4.14: Drain-actuated 3-terminal WALD NEMS switch FEM simulation; Model dimensions: 4,000 x 500 x 32 nm (S), $D_W = 250$ nm, $G_W = 1.875$ um (x2), $g_{DS} = 20$ nm, $g_{GS} = 50$ nm; $V_{Pullin} = 2.88$ V
Figure 4.15: Gate-actuated 3-terminal WALD NEMS switch FEM simulation; Model dimensions: $4,000 \times 500 \times 32 \text{ nm (S)}$, $D_W = 250 \text{ nm}$, $G_W = 1.875 \text{ um (x2)}$, $g_{DS} = 20 \text{ nm}$, $g_{GS} = 50 \text{ nm}$; $V_{Pullin} = 3.24 \text{ V}$

Figure 4.16: Drain-actuated 3-terminal WALD NEMS bow-tie switch FEM simulation; Model dimensions: $L = 4,000 \text{ nm}$, $W_M = 3.5 \text{ um}$, $W_o = 0.25 \text{ nm}$, $t = 32 \text{ nm}$, $D_W = 250 \text{ nm}$, $G_W = 1.875 \text{ um (x2)}$, $g_{DS} = 20 \text{ nm}$, $g_{GS} = 50 \text{ nm}$; $V_{Pullin} = 2.9 \text{ V}$
Figure 4.17: Gate-actuated 3-terminal WALD NEMS switch FEM simulation; Model dimensions: 4,000 x 500 x 32 nm (S), $D_W = 250$ nm, $G_W = 1.875$ um (x2), $g_{DS} = 20$ nm, $g_{GS} = 50$ nm; $V_{Pullin} = 1.48$ V

Figure 4.18: Comparison of FEM and theoretically calculated detachment curves
Figure 4.19: Gap Height Vs. $W_M$ for varying lengths of bow-tie structures; Dimension proportions: $D_W = .06L$, $W_o = 0.05L$, $t = 32$ nm
Figure 4.20: Bow-tie Detachment Study: (a) $\alpha$ Vs. Length; (b) $\beta$ Vs. Length; $\alpha$ was found to be quadratically dependent on L, and $\beta$ was found to be constant for all parameters.
Figure 4.21: Detachment curve for a WALD NEMS bow-tie device with variation of $W_M$ using equation 4.75
Chapter 5

Design, Development, and Fabrication of WALD NEMS devices

5.1 Overview

The following chapter chronicles the design, development and fabrication of several different WALD NEMS switches. The WALD NEMS devices presented in this chapter are as follows: 2-terminal fixed-fixed and cantilever switches with source-to-gate gap-heights of 50 nm, entrenched 2-terminal fixed-fixed switches with source-to-gate gap-heights of 30 nm, and a variety of entrenched 3-terminal fixed-fixed and cantilever switch designs. The 3-terminal switches presented in this chapter have source-to-gate gap heights of 65-50 nm, drain-to-source gap-heights of 20-15 nm, and rectangular, bow-tie, or poly-tie profiles.

The development of these devices resulted in the creation of 3-different novel, top-down, low-temperature, and CMOS integrable fabrication technologies, using for the first time ALD tungsten (WALD) as the primary structural material in a MEMS or NEMS device. While for this research effort the fabrication processes developed employed WALD as the structural material, they could be easily generalized for the fabrication of any thin-film NEMS device with out-of-plane functionality. Furthermore the technology developed for entrenched devices can easily be extended to accommodate the fabrication of novel n-terminal devices. N-terminal devices could potentially be developed as novel high-density memory or logic elements.

Finally, the fabrication results for each device fabricated are presented. The success and failures of each process/device will be discussed. As will be seen, the failure and success
of each process motivated the development of subsequent processes.

All of the work presented in the following two chapters, excluding details regarding WALD CNEMS inverters, has previously been reported by [53, 136, 109, 168, 110].

5.2 Elementary Analytic Stress Analysis for Simple Devices

Upon starting my graduate work at the University of Colorado I spent 9 months working with Dr. Y.J. Chang as he finished his dissertation. During that time we worked to develop the fabrication process described in section 5.3. From that work devices with working gaps of 100 nm were fabricated and characterized. These devices are referenced in section 5.2, and were the stepping-stone for my own work encompassed in this dissertation. For more detail about these devices please see Dr. Chang’s dissertation [37].

During pull-in testing of the NEMS cantilever devices with 100nm gap, failure was observed after a low number of cycles – typically 5-10 cycles. From IV measurements it was observed that when the devices failed they shorted to the actuation electrode/s. During IV characterization large negative shifts in pull-in voltage were observed until failure. For example, the initial pull-in voltage of the devices was found to be \(\sim 15\text{--}17\) Volts, but measured pull-in voltages just a few cycles later were measured to be as low as 5 Volts before failure. These large shifts indicate that the devices experienced some degree of plastic deformation upon actuation, which increased in subsequent actuation cycles. While designing the 100 nm generation of WALD devices, induced stresses were not considered, instead the design focused on pull-in voltage and detachment parameters, which are discussed detailed chapter 3 sections 3.3 and 3.4.4. Thus it became obvious that to engineer a successful thin-film device an adequate model for stress must be used in the design process. The device studied has dimensions 1300 x 700 x 30 nm (length x width x thickness), with a gap height of 100 nm. By modeling the device as a cantilever beam fully constrained at the anchor, and assuming that at the initial point of contact – the instant when the end of the beam makes contact with the drain electrode – the force acting on the beam is equivalent to a point load acting
on the tip of the device, we can determine the maximum moment acting on the device and thus the maximum internal stress of the beam.

For the aforementioned device this entails evaluating the following equation at $L = 1300$ nm and solving for the point load $F$.

$$g(x) = \frac{Fx^2(Ll - x)}{6EI}$$

(5.1)

For a cantilever beam the maximum moment acts at the anchor, and is equivalent to the product of the point load, $F$, that we assume is forcing the beam to contact the drain electrode, and the length of the beam. Through this analysis we arrive at an expression for the stress in the beam at the anchor,

$$\sigma(x) = \frac{6Eg(x)Ly}{x^2(3L - x)}_{x=L}$$

(5.2)

Here, $g(L)$ is the gap height of the device, for these devices equal to 100 nm. Via this equation we arrive at the conclusion that during actuation our devices experience an internal normal stress of at least 1,092 MPa. The yield stress of bulk tungsten is approximately 760 MPa; therefore, we quantitatively estimate that during each-cycle of operation a cantilever device with the given geometry and boundary conditions will experience plastic deformation.

### 5.2.1 Discussion

Plastic deformation has deleterious effects on the performance of the devices. Two possible causes of failure have been observed. The spring constant, and therefore restoring force, is directly affected by the plastic deformation near the anchor of the device. Because failure via stiction was not observed after the first couple of cycles for the 100 nm generation of devices, we can conclude that when the WALD structure was in contact with the drain electrode secondary bonding forces were not the dominate forces acting on the system, but as the device experienced plastic deformation during after repetitive cycling the secondary
forces began to dominate the weakened restoring force, resulting in a failure via stiction.

As previously mentioned it was observed that after each switching cycle the pull-in voltage decreased. If the devices are approximated to be parallel plate capacitors, we see that the pull-in voltage is a function of spring constant, $K$, and gap height, $g$:

$$V_{\text{pullin}} = \frac{2g}{3} \sqrt{\frac{2Kg}{3\varepsilon A}} \quad (5.3)$$

When the material experiences permanent strain in the actuated position, and is then released, the device retains some permanent deflection towards the substrate. Thus the observed shift in pull-in voltage can be attributed to the coupled effects of decreased stiffness and decreased gap height of the device – both consequences of plastic deformation. It should also be mentioned that other device properties, such as natural frequency, which depend on the stiffness, would also suffer from the effects of plastic deformation. The effect of plastic deformation would result in an observable negative shift in natural response and a decrease in the quality factor.

### 5.3 1st Generation 2-terminal WALD NEMS Switches

From the above stress analysis using elementary beam theory two new device geometries for both a cantilever and bridge type device were chosen. Both devices have were designed to have a 50 nm gap between the device and actuation electrode. The chosen dimensions for the cantilever devices were $1300 \times 700 \times 30$ nm, and $2,000 \times 700 \times 30$ nm for the bridge type devices. According to elementary beam theory, devices of these dimensions should undergo no plastic deformation, and thus no softening of the device effective stiffness should result from actuation. This analysis is based on the assumption that WALD material properties are the same as bulk W material properties (the mechanical material properties of WALD have yet to be studied). Because it had been observed that the initial restoring force in current devices is greater than the secondary forces during contact, it was expected that the redesigned devices should not suffer from low-cycle failure.
5.3.1 1st Generation WALD NEMS Fabrication Process (50 nm gap-heights)

The WALD NEMS devices reported here are designed to be electrostatically actuated relays/switches. The simplest design, with out-of-plane functionality, consists of an WALD nano-structure suspended over an actuation electrode. When a bias is applied between the ALD structure (source) and the actuation electrode (gate), they act as a capacitor, storing charge on their surfaces, thereby creating an electric field and associated electrostatic force. The resulting force bends the deformable ALD structure towards the substrate until the non-linear electrostatic force overcomes the restoring (spring) force, at which point the structure snaps-through making contact with the actuation electrode, closing the electric circuit. A derivation of the electrostatic force and pull-in voltage is given for a lumped model in chapter 3 section 3.3, and the snap-through phenomena is clearly illustrated by the phase-diagrams constructed during the non-linear system stability analysis described in chapter 3 section 3.4.3.

The fabrication process is shown in figure 5.1. The developed fabrication process for nano-scale WALD structures is a top-down approach based on MEMS surface micro-machining techniques. A silicon substrate with a 300 nm thermal oxide dielectric layer is coated by a 1.8 \( \mu \)m thick layer of AZP 4210, which is then patterned by photolithography to define alignment marks for the electron-beam (e-beam) lithography steps. After patterning the photo-resist, 50 nm of gold (Au) are deposited by thermal evaporation, and the alignment marks are defined by lift-off.

Next, the substrate is coated with a 150 nm thick layer of PMMA, and the device actuation electrodes are patterned by e-beam lithography. The 10 nm Au electrodes are then formed by thermal evaporation and lift-off. Following the electrode lift-off, a 50 nm thick sacrificial nickel (Ni) layer (this layer defines the air gap between the device and electrodes) is thermally evaporated, and then 2 nm of ALD alumina (Al2O3) and 30 nm ALD tungsten (W) are grown at a temperature of 120\(^\circ\) C on the top surface of the substrate. The metallic
Ni layer serves as the sacrificial layer and as the electrical connection between the gold layer underneath and the ALD structure.

The substrate is then coated by a 150 nm thick layer of PMMA, and next is patterned using e-beam. A hard mask used to define the geometry of the device is created after lift-off of a 20 nm thick thermally evaporated Ni layer. The ALD structures are defined after etching the WALD and alumina layers via RIE. A 100 nm thick layer of Au is next thermally evaporated and defined by lift-off. This layer creates large electrodes that connect to the actuation electrodes allowing for probing, and if made thicker, wire bonding. The substrate is then immersed into nickel etchant (Nickel Etchant TFB, Transene, USA) for 2 minutes to both release the structures and remove the hard mask. Finally, a CO$_2$ critical point dryer is used to prevent device stiction upon release.

5.3.2 1$^{st}$ Generation WALD NEMS 2-Terminal Fabrication Results

Two terminal WALD trench structures were successfully fabricated, figures 5.2 and 5.3. Figure 5.2 shows a successfully fabricated 2-terminal WALD NEMS cantilever device having dimensions 1,300 x 700 x 32 nm with a source-to-gate distance of 50 nm. Figure 5.3 shows a successfully fabricated 2-terminal WALD NEMS fixed-fixed device having dimensions 2,000 x 700 x 32 nm with a source-to-gate distance of 50 nm. For all WALD depositions thickness was confirmed via XRR measurement.

5.4 FEM Stress Analysis and Re-design

Testing and characterization of the 1$^{st}$ generation of devices (chapter 6) proved that the simple analytical analysis based on elementary beam theory was a good starting point for stress analysis, but not a completely adequate one. The theory’s main fault is its inability to account for stress after snap-through of the device. At snap-through a large percentage of the total overlap area between the device and actuation electrode comes into contact, figure 6.9b. When this happens stress in the device drastically increases. Thus finite element models are
Figure 5.1: WALD NEMS Fabrication Process for 2-Terminal Devices with 50 nm Gaps

1. Apply AZP 4210 to [100] Si Wafer with a 300 nm thick layer of thermal oxide

2. Pattern AZP 4210, evaporate 50 nm Ti/Au for alignment marks

3. Perform lift-off to define e-beam alignment marks, apply PMMA

4. Pattern electrode geometry via e-beam lithography, evaporate 10 nm Ti/Au

5. Perform lift-off to define electrodes, evaporate 50 nm Ni and grow 32 nm WALD

6. Apply PMMA, pattern WALD structure geometry via e-beam lithography, evaporate 30 nm Ni hard mask

7. Perform lift-off to define hard mask, pattern WALD in RIE

8. Apply and pattern AZP 4210, evaporate 100+ nm of Ti/AU for bonding/probing pads

9. Perform lift-off to define pads, etch WALD in RIE, release WALD structure via wet Ni etch dry in CO2 dryer

PMMA | AZP 4210 | Au | WALD | Ni
required to properly characterize and design reliable NEMS switches. Using ANSYS, our 2-terminal device WALD device has been modeled to study the stress induced in the device at the point of initial contact as well as after snap-through.

First a model was created having the same dimensions as the fabricated 1st generation 2-terminal devices (2000 x 700 x 30 nm, and electrode area 1000x 700 nm²). Two different models were created. The first models the device at the initial point of contact, and the second models the device at snap-through. It was assumed that at snap-through the device made full contact with the entire surface area of the actuation electrode. The boundary conditions for all of the FEM models were displacement conditions. The anchors were fixed in a pinned-pinned manner, meaning that rotation of the anchors was allowed but displacement in any of the Cartesian directions was fully constrained. A multi-physics model was avoided.
by applying a displacement to the device corresponding to the desired deflection during operation. The purpose of two models was to gain insight into the effect of the snap-through geometry on stress in the device.

The models are shown in figure 6.9a,b. It was found that at the point of initial contact the maximum Von Mises stress in the device was 2,791 MPa, and after snap-through the Von Mises stress increased to 8,390 MPa, a factor of 3. Von Mises stress, which is essentially an RMS average of the principle stresses at a point, is an excellent method for predicting the onset of plastic failure. If the Von Mises stress exceeds the yield stress of the material then the device has failed. The yield stress of tungsten is 760 MPa, therefore it is clear that even before initial contact between the device and gate electrode is made, the fabricated 50 nm WALD devices experience permanent deformation during operation.

Because FEM analysis revealed that the fabricated 50 nm devices failed during operation, new FEM models were created to aid in the design of a geometry that would produce reliable devices having 50 nm gaps. Using FEM analysis several different geometries based on a change in device length were considered. Their results are summarized in figure 5.6 (the figure also contains information regarding the theoretical pull-in voltage expected for each design).

The design iteration with the device length increased to 4 um illustrates the importance of modeling both initial contact and snap-through contact using FEM as an aid for design. In figure 5.5a the device is shown at initial contact with the actuation electrode, and the maximum Von Mises stress is found to be 709 MPa, which is less than the failure criterion of 760 MPa for bulk tungsten, but in figure 5.5b we see that at snap-through the maximum Von Mises stress has increased to 1,118 MPa implying plastic failure. This example reveals that although the modeled device is capable of deflecting the full 50 nm to make contact with the electrode, it is not able to accommodate contact experienced after snap-through.

Figures 6.9 and 5.5 reveal that during initial contact the maximum Von Mises stress in the device is found at the anchors, which is the same result predicted by elementary
Figure 5.4: Initial contact of a 2000x700x30nm WALD device, scaling 5x; Snap-thru contact of a 2000 x 700 x 30 nm WALD device, scaling 5x
Figure 5.5: Initial contact of a 4000 x 500 x 30 nm WALD device, scaling 5x; Snap-thru contact of a 4000 x 500 x 30 nm WALD device, scaling 5x
Figure 5.6: FEM stress analysis for different WALD device geometries, and theoretical and experimental pull-in voltages (if available).

beam theory. However, when the device is in full contact with the actuation electrode, the region of highest stress shifts to either the edge or the actuation electrode where the device geometry shifts, in a point-wise fashion, from being deflected at some angle to being completely parallel with the substrate. This stress concentration proved to be important for future design considerations of WALD NEMS fabrication processes.

It was observed that the location of highest stress predicted by the FEM stress analysis corresponded exactly to the point of failure for 1st generation devices. This particular location happened to coincide with a fabrication induced stress concentration, resulting from a non-ideal conformal coating of sacrificial and structural layers over the lift-off defined actuation electrode. The induced stress concentration proved to be a limiting factor regarding the minimum achievable gap heights and minimum thickness of the WALD film able to be used in the design of WALD NEMS switches. It was shown via the FEM analysis that by increasing the length of the device, or decreasing the source-to-gate gap height, the induced stress could be minimized. Thus, the limitations of this fabrication process implied that the process was not capable of producing reliable WALD NEMS devices. For this reason a new fabrication process was developed to remove any and all stress concentrations induced by the 1st generation fabrication process, thereby producing reliable WALD NEMS switches.


5.5 2nd Generation 2-Terminal WALD NEMS Switches (Entrenched Devices)

The development of the previous generation of fixed-fixed 2-terminal devices having nominal source-to-gate gap heights of 100 and 50 nm revealed several limitations inherent in the developed fabrication process that would severely limit research progress if not addressed. First, it was found that the lift-off process used to create the source/drain electrodes limited the gap height. This was discovered when attempting to create devices with nominal gap heights of 30 nm. The sharp features along the actuation electrodes, seen in figure 5.2, were observed to propagate through the sacrificial layer and appear in the WALD, thus regions of high stress were created in the functioning structure. Upon release the structures failed at these locations. Second, testing on both the 100 and 50 nm devices showed very low switching lifetimes. To produce reliable devices without increasing the device dimensions the most obvious solution is to decrease the gap height, but because the gap height was limited by the lift-off process this was not possible. Finally, the process proved to be impractical for the fabrication of 3-terminal bridge devices, because of the inability to create a raised drain electrode to prevent shorting with adjacent and coplanar gate electrodes. With the development of a new process, based on that of the 1st generation process, all of the aforementioned limitations of the 1st generation process were sufficiently addressed. In doing so, a fabrication process capable of producing two and 3-terminal devices, whose gap-heights are limited only by deposition technique, was successfully developed.

To circumvent the problems caused by the sharp features created during lift-off a fabrication technique was developed to deposit the electrode in a trench etched via RIE into the thermal oxide layer. This technique effectively eliminated the problems caused by lift-off and allowed for the creation of source-to-gate gaps limited only by the conformity of the deposition technique used to deposit the sacrificial material. Furthermore, in this process, because the actuating electrode is electrically isolated from the device (source),
an electrode/device overlap area of 100% can be achieved. In the 1st generation process
electrical isolation was achieved by creating a gap between the actuation electrode and Ni
used to anchor the WALD structure to the substrate. Using this process gaps as small as 30
nm were fabricated, and the switching behavior of those devices successfully characterized.
Finally, because the process places electrodes inside of a trench it is possible to create a raised
drain electrode within the trench that is also electrically isolated from a gate electrode. In
this way the process may be extended for the development of 3-terminal devices, necessary
for the construction of complementary mechanical logic. This extension is detailed in the
following section 5.6.

5.5.1 2-Terminal WALD Entrenched NEMS Fabrication Process

The fabrication process is shown in figure 5.7. The developed fabrication process
for nano-scale WALD structures is a top-down approach based on MEMS surface micro-
machining techniques and sacrificial layering techniques developed for the 1st generation
(100/50 nm gap heights) WALD devices. A silicon substrate with a 300 nm thermal oxide
dielectric layer is coated by a 1.8 $\mu$m thick layer of AZP 4210, which is then patterned by
photolithography to define alignment marks for electron-beam (e-beam) lithography steps.
After patterning the photoresist, 50 nm of gold (Au) is deposited via thermal evaporation,
and the alignment marks defined through lift-off.

Next, the substrate is double coated by two layers of PMMA, each layer having a
thickness 500 nm. The first layer is spun on and the chip soft baked for 2 minutes at 120$^\circ$
C, then the second layer is spun on followed by a hard bake for 10 minutes at 170$^\circ$ C. This
creates a layer of PMMA having a nominal thickness of 1 $\mu$m. A relatively thick layer of
PMMA is needed so that a sufficiently thick layer of PMMA remains on the chip after RIE.
The device electrodes are patterned by e-beam lithography. A 50 nm trench is created in the
thermal oxide layer using RIE. A stack of metals is then deposited over the chip by thermal
evaporation. A 5 nm thick adhesive layer Ti is deposited followed by a 15 nm thick layer of
Au and a 30 nm thick sacrificial layer of Ni.

Following deposition of the metal stack, lift-off leaves the metal layers filling only the trench. Next, 2 nm of ALD alumina ($\text{Al}_2\text{O}_3$) and 30 nm WALD are grown at a temperature of 120° C over the substrate. Then the substrate is coated by a 150 nm thick layer of PMMA and patterned using e-beam to create device geometries. A 30 nm thick thermally evaporated Ni layer is deposited creating hard mask used to define the geometry of the devices during RIE. The ALD structures are defined after etching the WALD and $\text{Al}_2\text{O}_3$ layers using RIE. A 100 nm thick layer of Au is thermally evaporated and defined by lift-off. This layer creates large electrodes that connect to the actuation electrodes, allowing for probing, and if made thicker, wire bonding.

Finally, the substrate is immersed into nickel etchant (Nickel Etchant TFB, Transene, USA) for $\approx$ 30 seconds, releasing the structures and removing the hard mask. After release a $\text{CO}_2$ critical point dryer used to prevent device stiction upon release.

5.5.2 2-Terminal WALD Entrenched NEMS Fabrication Results

Two-terminal WALD trench structures have been successfully fabricated, figure 5.8. Figure 5.8a shows a 3-D CAD model of the designed device. Figures 5.8b,c show a successfully fabricated 2-terminal WALD trench NEMS device having dimensions 3,000 x 500 x 30 nm and an air gap of 30 nm. The thickness of WALD thin film was confirmed by the XRR measurement. The depth of the trench was confirmed via focused ion beam (FIB). Several measurements were made, and an average trench depth was calculated to be $\approx$ 100 nm, shown in figure 5.8d. In figures 5.8b-d it appears that there may be contaminants on the substrate. Because of this, the devices were placed in oxygen plasma RIE before characterization.

5.6 Entrenched 3-Terminal WALD NEMS Switches

After the successful development of entrenched 2-terminal WALD NEMS switches the focus of the research effort turned to the development of 3-terminal WALD NEMS
Figure 5.7: Fabrication Process for 2nd generation 2-terminal WALD NEMS devices
switches. Following the successful development of the 2nd generation of 2-terminal devices, the approach chosen for the development of reliable 3-terminal WALD NEMS switches was to extend the fabrication process developed for the 2nd generation of 2-terminal WALD NEMS switches. The fabrication process that was developed is novel and exciting. The 3-terminal fabrication process extends that of the 2-terminal WALD entrenched NEMS devices by furthering the use of embedded electrodes.

In this process the gate electrode is created as before, but a drain electrode is now embedded in the substrate. The drain electrode is deposited in an RIE etched trench that is shallower than that of the gate electrode. This technique keeps the source and drain
electrodes electrically isolated, enabling gate controlled 2-terminal switching as opposed to shunt switching. The development of these devices theoretically allows for the construction of mechanical logic devices because fundamental logic devices analogous to CMOS inverters can be constructed by connecting multiple 3-terminal devices together via common gate and drain electrodes, as was most recently demonstrated by [136].

5.6.1 Entrenched 3-Terminal WALD NEMS Fabrication Process

The 3-terminal process presented here is an extension of the 2-terminal WALD entrenched NEMS fabrication process first introduced in [52] and summarized in detail in section 5.5.1. This process furthers the use of entrenched electrodes, demonstrating the process’ utility in the fabrication of multiple electrically isolated electrodes with different gap heights. Here gate electrodes are fabricated as described in section 5.5.1, but now a drain electrode is also entrenched. The drain electrode and gate-electrode are electrically isolated via a 10-15 nm thick layer of $SiO_2$, which results from the two entrenching processes.

The fabrication process is shown below in figure 5.9. The developed fabrication process for 3-terminal nano-scale WALD devices is a top-down approach based on MEMS surface micro-machining techniques and sacrificial layering techniques developed earlier and first reported in [54, 52]. Initially a silicon substrate (100) with a 300 nm dielectric layer of thermal oxide is coated by a 1.8 $\mu$m thick layer of AZP 4210 and patterned by photolithography to define alignment marks for electron-beam (e-beam) lithography steps. After patterning the photo-resist, a 50 nm thick layer of gold (Au) is deposited by thermal evaporation, and alignment marks defines by lift-off.

In steps 1-2 the substrate is double-coated by two 500 nm thick layers of PMMA. The first layer is spun on and the chip soft-baked for 2 minutes at 120$^\circ$ C, then a second layer is spun on followed by a hard-bake for 10 minutes at 170$^\circ$ C. This creates a thick layer of PMMA with a nominal thickness of 1 $\mu$m. Next, the device’s gate electrodes are patterned via e-beam lithography. A 75 nm deep trench is created in the thermal oxide layer using
RIE with a 4:1, $CF_4:O_2$ chemistry. Finally, a stack of metals is deposited in the trench via thermal evaporation to form the gate electrodes and sacrificial layer between the gate electrodes and WALD structure. The stack is composed of a 5 nm thick adhesion layer of Ti, followed by a 20 nm thick layer of Au, and a 50 nm thick sacrificial layer of Ni. Following deposition of the metal stack, lift-off leaves the metal layers filling only the gate trench.

In step 3-4 the process is repeated to create the drain electrode. Again, the substrate is double-coated with two layers of PMMA, and the drain electrode patterned via e-beam lithography. A 40 nm deep trench is created in the thermal oxide layer via RIE. A stack of metals is again deposited on the chip by thermal evaporation to form the drain electrode and sacrificial layer between the drain and WALD structure, which includes: a 5 nm thick adhesion layer of Ti, followed by a 15 nm thick layer of Au, and a 20 nm thick sacrificial layer of Ni. Following lift-off, 2 nm of ALD $Al_2O_3$ and 30 nm WALD are grown on the substrate at $120^\circ$ C.

In steps 5-6 the substrate is coated by a single layer of PMMA, and patterned via e-beam to create the device geometries. Next, a 30 nm thick thermally evaporated Ni layer is deposited, creating hard mask used to define the geometry of the devices during RIE. In step 7, the WALD structures are developed after etching the ALD via RIE. After RIE, 300 nm thick Au electrodes for probing and wire bonding are defined by optical lithography, thermal evaporation, and lift-off. In step 8 the substrate is immersed into nickel etchant (Nickel Etchant TFB, Transene, USA) for up to 5 minutes to remove the hard mask and sacrificial layers. Finally, the chips are placed in a $CO_2$ critical point dryer to prevent stiction upon release.

5.6.2 Entrenched 3-Terminal WALD NEMS Switches/Transistors Fabrication Results

Fabrication results are shown in figures 5.10b-c. Figure 5.10a shows a CAD representation of the initial design for the 3-terminal WALD NEMS switches. Figure 5.10c shows
the fabricated device at 1,750X; in the figure, the device, as well as surrounding bonding pads are visible. The gate electrodes, which are seen as the deeper trench (starting at the bottom of the frame), are both designed to have electrode/device overlap areas of 1,250 x 500 nm with a gap of 50 nm between electrode and device. The drain electrode, centered
beneath the device, is designed to have an electrode/device overlap area of 500 x 500 nm with a gap of 20 nm between electrode and device. Figure 5.10c shows the same device at 12,500X, focusing only on the device. Here an appreciable amount of overlap between the gate and drain electrodes is visible.

Figure 5.10: 3-D model and SEM images of 3-terminal WALD NEMS switch; Designed Dimensions: (S) 3,000 x 500 x 32 nm, (D) 7,00 x 500 nm, (G) 1,250 x 500, gap$_{DS}$ = 20 nm, gap$_{GS}$ = 50 nm

### 5.7 Redesign of 3-terminal WALD NEMS Switches

The 3-terminal WALD NEMS switches fabricated were considered to be largely a success. A number fabricated devices were shown to function properly via switching char-
acterization, however it was observed that an unacceptable percentage of fabricated devices
failed either prior to, or upon, actuation (chapter 6). A device is considered to have failed
prior to actuation when it’s gate and drain electrode are electrically shorted together. A
device is considered to have failed upon actuation if current is measured between gate and
source electrodes, which indicates that at pull-in the source snaps-thru to the gate electrode,
thereby shorting the gate to the drain. A CAD representation of this event is shown in figure
5.13. These issues were sufficiently addressed through detailed study of key elements of the
fabrication process and subsequent redesign of device geometries.

5.7.1 Minimization of Over-etching and Associated Gate/Source Overlap

The most likely cause of pre-actuation shorting between gate and drain electrodes was
the undesirable overlap of the electrodes, clearly seen in figures 5.10 b,c. Initially it was
thought that the overlap may be a result of a low quality e-beam write, or possibly due
to the anisotropy of the RIE, but upon further research into the problem these theories
were rejected. Citing [220], it was found that the gate/drain electrode overlap – apparently
resulting from over-etching of trenches prior to metal deposition (steps 1-4, section 5.6.1)–
actually resulted from electron-scattering induced cavitation of the PMMA.

In [220] an excellent schematic of the standard e-beam/deposition/lift-off process com-
monly used in nano-fabrication is given, figure 5.11. In 5.11a electron beam injection with
scattering is illustrated. Figure 5.11b shows a cross-section of the developed resist. In it we
see that the scattered electrons develop a region around the intended pattern as they pene-
trate the resist. This material is removed by the developer, which results in a cavity within
the resist. Figures 5.11c, and d illustrate the remainder of the deposition/lift-off process.

In these illustrations it is seen that the intended pattern (a rectangle) is properly
developed on the surface of the resist, with the cavity opening up below. Therefore if material
is deposited via a PVD process (thermal evaporation, sputtering, e-beam evaporation etc),
the developed mask produces a rectangular feature on the substrate as desired. Because the
The cavity is shielded by the rectangular opening it has essentially no effect on fabrication of the intended structure.

The standard e-beam/deposition/lift-off process described by [220] is used for all e-beam steps in the 1st generation 2-terminal WALD NEMS fabrication process, section 5.3.1, and develop the hard Ni masks used to define the WALD structures for both of the entrenched WALD NEMS process, sections 5.5.1 and 5.6.1. Therefore, unless the e-beam gun is poorly focused, one would not expect any noticeable variations between the designed and fabricated geometries for these steps, as was the case. However, the gate and drains electrodes for entrenched 2 and 3-terminal devices are not fabricated using the standard e-beam/deposition/lift-off process described above.

As was described in sections 5.5.1 and 5.6.1 the electrodes are developed using a novel e-beam/RIE/deposition/lift-off technique. The first issue with this technique is the resist thickness. Typically only a very thin coat of resist is required, or desirable, for e-beam lithography, but in the fabrication processes developed here the resist has to be thick enough such that it is not removed during RIE and after RIE it maintains a sufficient thickness as to allow for metal-deposition and lift-off. For this reason, both entrenching processes use a double-coated layer of PMMA that was measured to be 1 μm thick using a surface profilometer. Now, the patterns that are written via e-beam into the double-thick PMMA have minimum lateral dimensions that range from 0.5 to 1.725 μm, implying a resist-to-geometry ratio of 2 to 0.58. For such geometries and ratios the effects of electron scattering in the resist, and thus cavitation, should therefore be considered significant.

The next issue with the e-beam/RIE/deposition/lift-off technique is the RIE step. In the standard e-beam/deposition/lift-off technique the cavity has no effect on the geometry of the deposited structure, but this is not true when RIE is introduced before deposition. The RIE chemistry used in these processes (4:1, $CF_4:O_2$) is isotropic. This implies that as the trench geometry is etched into the $SiO_2$, the PMMA mask and associated cavity are laterally etched, resulting in the effective widening of the mask, cavity, and etched trench.
After RIE the metals that compose the electrodes as well as sacrificial layer are deposited via thermal evaporation, however the PMMA mask has now been widened, thus resulting in the over-etched/overlapping electrode geometries visible in figure 5.10b,c.
5.7.2 Characterization of Cavitation Effects

To minimize the effects stemming from the e-beam/RIE/deposition/lift-off steps used in the entrenched WALD NEMS processes, the steps were characterized quantitatively. Because direct measurement of the cavity would prove to be difficult and time consuming, and because the effect of RIE is coupled to the initial cavity size and patterned geometry, the effect of cavitation and isotropic etching on the variation of fabricated geometry versus intended geometry was studied by measuring electrode and total device widths post deposition/lift-off. This study was accomplished using SEM images of devices fabricated during 2008 and 2009. These chips included entrenched 2-terminal switches and two different designs of 3-terminal switches. Measurements were taken using ImageJ, a free image processing package that can be used for transforming number of pixels to physical distance/area.

The results of this study are summarized in tables 5.1-5.3. From this data the average rate that a structure was over-etched was determined. It was found that by lumping the effects of cavitation and isotropic etching, the over-etch rate was on average $7.36 \pm 0.39 \text{ nm/s}$ for the gate electrode of 2-terminal devices, $1.84 \pm 0.09 \text{ nm/s}$ for the gate electrodes of 3-terminal devices, and $2.09 \pm 0.22 \text{ nm/s}$ for the drain electrodes of 3-terminal devices. Using these average average rates, masks can be created to completely compensate for the deleterious effects of cavitation and isotropic etching on intended electrode geometries developed by e-beam/RIE/deposition/lift-off steps. This is demonstrated in section 5.7.4.

Table 5.1: 2-terminal WALD NEMS Switch Design: Fall 2008

<table>
<thead>
<tr>
<th>As Designed</th>
<th>$l_o = 3000 \text{ nm}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabricated Length</td>
<td>$3883.3 \pm 47.226 \text{ nm}$</td>
</tr>
</tbody>
</table>
Table 5.2: 3-terminal WALD NEMS Switch Design: Spring 2009

<table>
<thead>
<tr>
<th>As Designed</th>
<th>$(l_o, gw_o, dw_o) = (3000, 1250, 500)$ nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabricated Length</td>
<td>$3374.1 \pm 77.247$ nm</td>
</tr>
<tr>
<td>Fabricated Gate Width</td>
<td>$1543.7 \pm 26.845$ nm</td>
</tr>
<tr>
<td>Fabricated Drain Width</td>
<td>$1060.7 \pm 68.921$ nm</td>
</tr>
</tbody>
</table>

Table 5.3: 3-terminal WALD NEMS Switch Design: Summer 2009

<table>
<thead>
<tr>
<th>As Designed</th>
<th>$(l_o, gw_o, dw_o) = (4000, 1750, 500)$ nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabricated Length</td>
<td>$4462.3 \pm 25.594$ nm</td>
</tr>
<tr>
<td>Fabricated Gate Width</td>
<td>$2146.1 \pm 43.283$ nm</td>
</tr>
<tr>
<td>Fabricated Drain Width</td>
<td>$701.28 \pm 19.371$ nm</td>
</tr>
</tbody>
</table>

5.7.3 Shorting Between Gate and Drain at Pull-in

While IV characterization of three-terminal WALD 3-terminal switches was largely successful, one recurring flaw in the devices was observed which limited device reliability. Frequently during IV characterization the measured $I_{DS}$ current mirrored the measured $I_{GS}$ current, e.g., $|I_{DS}| = |I_{GS}|$. A set of IV curves for a WALD 3-terminal switch showing the mirrored currents is given in figure 5.12. Because $I_{DS}$ and $I_{GS}$ have the same magnitude but opposite sign, and $I_{DS} > 0$, we know that current flows to the parameter analyzer via the drain terminal. We also know that current flows away from the parameter analyzer as measured from the gate terminals because $I_{GS} < 0$. This indicates that the source has shorted across both the drain and gate terminals, as illustrated in figure 5.13. The shorting event is undesirable if the 3-terminal switch is to operate properly in an inverter system.

5.7.3.1 The Shorting Solution

When the center of the 3-terminal device makes contact with the drain, it essentially becomes two preloaded 2-terminal devices each having a source-to-gate gap height of $\sim 30$ nm – the gap height difference between the gate and drain electrode. Because the actuating
Figure 5.12: IV curves demonstrating a short between drain and gate electrodes upon actuation, $I_{DS}$ mirrors $I_{GS}$ for corresponding $V_{GS}$ indicating a short upon actuation, current is limited to 300 nA.

Figure 5.13: FEM model demonstrated snap-through of device over a narrow drain electrode voltage is not removed once contact between the source and gate has been made there exists what should be thought of as an undesirable post actuation electric field between the source and gates, and if this field is large enough the device snaps-thru to the gate electrode, shorting
the device, as illustrated in figure 5.13.

To solve this problem the width of the drain was increased and the width of the gate electrodes decreased. By doing this the length of the so called "pre-loaded" 2-terminal switches is shortened, increasing their respective effective stiffnesses, which in-turn increases the magnitude of the required electric-field necessary to pull the devices in to the gate electrode. Thus if the drain electrode is large enough it will effectively act as a mechanical stop, preventing shorting, and ensuring that the device operates reliably as a NEMS 3-terminal switch, illustrated in figure 5.14. Unfortunately, by decreasing the total overlap area between the source and gate the influence of the gate electrode during actuation is diminished.

![Figure 5.14: FEM model demonstrated snap-through of device over a wide drain electrode; the wider electrode helps prevent shorting between the gate and drain electrodes.](image)

5.7.4 Redesigned 3-terminal WALD NEMS Switches and Fabrication Results

Using the information garnered from statistically characterizing the coupled effects of e-beam induced cavitation and isotropic RIE on the 3-terminal WALD NEMS fabrication process, mask files were successfully designed to compensate for over-etching. Because it was determined via Student’s t-test that the characterized over-etch rates for the gate and drain electrode were not significantly different, only one over-etch rate was used to design
the mask files for gate and drain electrode geometries. For this purpose an over-etch rate of \( \approx 1.96 \text{ nm/s} \) was assumed. This is the average value of the over-etch rates calculated for the gate and drain electrode geometries of previously fabricated 3-terminal devices. Finally, this rate was deemed to be satisfactory because it falls within one standard deviation of both characterized gate and drain geometry over-etch rates.

5.7.4.1 Fixed-fixed Switches

To address the problem of shorting between the gate and drain electrodes at actuation, the length of the device was increased, the drain electrode width increased, and the gate electrode widths decreased. The overall length of the fixed-fixed beam was increased for two purposes. First, and simply enough, increasing the length of the device gives more room to work with. This way the width of the drain can be increased, and the width of the gates decreased, without potentially compromising the quality of fabrication. By this I mean if the gate electrode widths became too small because they were constrained by the overall length of a short source, then problems with minimum e-beam writable geometries might be experienced. From experience this means gate electrodes may not be fully formed, or if they are formed they are much wider than intended. This last case is a result of a large aspect ratio between the pattern width and e-beam thickness, as previously mentioned.

Second, by increasing the length of the source the pull-in voltage of the device is decreased. Furthermore, by allowing the reduced gate electrodes to be wider than they would be if scaled to a shorter source, the influence of the electrostatic load applied by the gate electrodes is improved. This way the gate actuated pull-in voltages should not be unreasonably large.

The exact geometries of the redesigned 3-terminal fixed-fixed WALD NEMS switch are given in table 5.4, and fabrication results are shown by figure 5.17.
Table 5.4: 3-terminal Fixed-fixed WALD NEMS Switch Geometries (wide drain)

<table>
<thead>
<tr>
<th>Feature</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source</td>
<td>4,000 x 500 x 32 nm</td>
</tr>
<tr>
<td>Gate (x2)</td>
<td>1,000 x 500 nm</td>
</tr>
<tr>
<td>Drain</td>
<td>2,000 x 500 nm</td>
</tr>
</tbody>
</table>

5.7.4.2 Cantilever Switches

The majority of the devices fabricated by this work were based on fixed-fixed bridge-type designs. However, at the start of this research effort cantilever devices were fabricated with using the 1<sup>st</sup> generation fabrication process presented in section 5.3, as first reported in[54]. Cantilever devices were not initially considered using later fabrication technologies, sections 5.5.1 and 5.6.1, because of several reliability concerns observed during characterization of 1<sup>st</sup> generation devices.

First, the devices appeared to suffer from appreciable residual stress, resulting in out-of-plane curvature that drastically increased expected pull-in voltages. Second, compared to fixed-fixed structures, the devices were observed to be more susceptible to mechanical failure at stress concentrations induced by the edges of the actuation electrodes. Furthermore, within 100 actuation cycles substantial shifts in threshold voltage were observed, with devices ultimately failing after welding to the actuation electrode, figure 5.15. However, it was recently reported by Czaplewski et al. that their TF NEMS cantilever switches also failed by welding. They reported that device reliability was substantially improved for devices coated by a thin layer of oxide. Therefore cantilever devices could be coated by a thin layer of ALD alumina to limit welding, and increase reliability. It should be noted that the failure mechanisms proposed by Czaplewski, which are the same that I initially suspected, namely, arcing caused by increased charge densities at the tip at pull-in [51], are of no consequence for fixed-fixed devices.

Cantilever switch designs have been successfully implemented in MEMS/ NEMS and
offer a distinct advantage over fixed-fixed structures. For a given geometry a cantilever is a softer structure, and thus has a lower actuation voltage. Because the fabrication technologies developed for entrenched WALD NEMS devices successfully removed stress concentrations produced by the 1st generation technology, and a potential solution to the previously identified failure mechanism has been proposed by Czaplewski et al. [51], cantilever designs for 3-terminal WALD NEMS switches were designed, fabricated and studied in parallel with the 3-terminal fixed-fixed WALD NEMS design just detailed.

The cantilever devices were designed using the same gate and electrode geometries designed for the 3-terminal fixed-fixed switch. These devices are designed such that the free end of the beam is suspended above the centrally located drain electrode. Because the cantilevers have a free end, two or more electrically isolated WALD cantilevers structures can be suspended above one set of electrodes. An example of this concept is illustrated in figure 5.16. For several different reasons the design for 3-terminal cantilever switches offers a great advantage of the that of the fixed-fixed devices. More devices per fabrication run can be fabricated, which results in more devices per run to be characterized, and most
importantly saves time and money. When considering device integration, this design has a much smaller footprint per device allowing for a higher device integration density. A higher device integration density may prove to be game changing for future CMOS/NEMS integrated devices. Finally, the design shown in figure 5.16 is theoretically** that of a complementary NEMS inverter.

The exact geometries of the 3-terminal cantilever WALD NEMS switch are given in table 5.5, and fabrication results are shown by figure 5.18.

Table 5.5: 3-terminal Cantilever WALD NEMS Switch Geometries (wide drain)

<table>
<thead>
<tr>
<th>Feature</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source</td>
<td>3,000 x 500 x 32 nm</td>
</tr>
<tr>
<td>Gate (x2)</td>
<td>1,000 x 500 nm</td>
</tr>
<tr>
<td>Drain</td>
<td>2,000 x 500 nm[1ex]</td>
</tr>
</tbody>
</table>

Figure 5.16: Example of an e-beam mask file for a 3-terminal cantilever WALD NEMS device

**WALD NEMS inverter design is discussed in detail next.
5.7.4.3 Fabrication Results

Fabrication results for the 3-terminal WALD NEMS switches redesigned to compensate for overetching (elimate gate drain overlap) and to prevent gate to drain shorting are shown in figures 5.17 and 5.18. As is evident by the SEM images the statistical characterization of the cavitation/RIE problem was a success. Compared to initially fabricated 3-terminal fixed-fixed WALD NEMS switches, figure 5.10, the electrodes of the devices shown here have no visually identifiable gate/drain overlap. Furthermore, these redesigned devices proved to be a complete success because, by increasing the width of the drain, shorting between the gate and drain was completely eliminated, as is reported in chapter 6.

Figure 5.17: SEM images of redesigned 3-terminal fixed-fixed WALD NEMS switch with wide drain; Designed Dimensions: (S) 4,000 x 500 x 32 nm, (D) 2,000 x 500 nm, (G) 1,000 x 500, gap_{DS} = 20 nm, gap_{GS} = 50 nm
Figure 5.18: SEM images of redesigned 3-terminal cantilever WALD NEMS switch with wide drain; Designed Dimensions: (S) 3,000 x 500 x 32 nm, (D) 2,000 x 500 nm, (G) 1,000 x 500, gap_{DS} = 20 nm, gap_{GS} = 50 nm

5.8 Design and Fabrication of Complementary WALD NEMS Inverters

WALD Complementary NEMS (CNEMS) Inverters have been designed using the 3-terminal WALD NEMS fabrication process described in section 5.6.1. The following section details the operating principle, design, and fabrication of these devices.

5.8.1 Operating Principle

The operating principle of a CMEMS/NEMS inverter is analogous to that of complementarily biased IC inverter. The inverter is constructed by two 3-terminal switches, analogous to transistors, with common gate and drain terminals. The inverter construction and biasing is shown by a circuit diagram in figure 5.19. The sources (suspended WALD structures) are then complementarily biased by V_{DD} = high and V_{SS} = low. As reported in chapter 2, this design has been successfully utilized for CMEMS inverters by Yakota et al.
[167, 236], and most recently for CNEMS inverters by Merhegeny et al. [136].

The operation of a CMEMS/CNEMS fixed-fixed type inverter is illustrated in figure 5.20 and summarized by a truth table 5.6. The given truth table also lists the switch positions required for operation. The switches are labeled ”A” and ”B” and correspond to the labeling of sources in the circuit diagram.

Although the operation and construction of a CMEMS/NEMS inverter are analogous to that of a complementary IC inverter, electrostatic actuation of MEMS/NEMS structures
Table 5.6: CMEMS/NEMS inverter truth table

<table>
<thead>
<tr>
<th>$V_{in}$</th>
<th>$V_{out}$</th>
<th>Switch A Position</th>
<th>Switch B Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>open</td>
<td>closed</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>closed</td>
<td>open</td>
</tr>
</tbody>
</table>

(sources) is fundamentally different from that of electric field operated transistors, and this results in a set of CMEMS/CNEMS specific design rules. Figure 5.20 shows an illustration of an operating CMEMS/NEMS inverter. In figure (a) we have the logical case $V_{in} = 1$ and $V_{out} = 0$. For this case $V_{GS} = V_{DD}$ (logical 1), $V_{S1} = V_{SS}$, and $V_{S2} = V_{DD}$, thus there exists some potential between the gate terminal and $S_1$, and zero potential between the gate terminal and $S_2$. Here we have assumed that the potential between the gate and $S_1$ is large enough to result in pull-in of $S_1$ to the drain terminal. Because the drain is left floating the drain terminal takes on the voltage applied to $S_1$ which is $V_{SS}$ (logical 0).

Now, in figure (b) we have the logical case $V_{in} = 0$ and $V_{out} = 1$. For this case $V_{GS} = V_{SS}$ (logical 0), $V_{S1} = V_{SS}$, and $V_{S2} = V_{DD}$, thus there exists some potential between the gate terminal and $S_2$, and zero potential between the gate terminal and $S_0$. As for case 1, we assume that the potential between the gate and $S_2$ is large enough to result in pull-in of $S_2$ to the drain terminal. Because the drain terminal is left floating the drain terminal takes on the voltage applied to $S_2$ which is $V_{DD}$ (logical 1).

It is this case that can result in potential failure of a CMEMS/CNEMS inverter. When the drain takes on voltage $V_{DD}$ the potential between the drain and $S_1$ becomes non-zero and is equal to $V_{DD} - V_{SS}$. This potential will result in an electric static load that will displace $S_1$ some distance towards the drain. If the potential is sufficiently small then the beam will reach some stable equilibrium point (section 3.4.3), and the device will operate as intended. However, if the induced potential is large enough $S_1$ will be actuated by $S_2$, resulting in a short between $S_1$ and $S_2$ and failure of the device.
5.8.2 FEM/FLFD Aided Design Study

5.8.2.1 Motivation for the Design Study

Based on the described operating principle, at first-glance it would that a CMEM-S/NEMS inverter can be constructed any identical pair of complementarily biased 3-terminal switches, and this was the initial approach taken by this research effort. The thinking was that because 3-terminal WALD switches had been successfully developed, WALD CNEMS inverters should immediately follow. As such, WALD CNEMS inverters were fabricated in parallel with 3-terminal WALD switches. Fabrication results are shown in figure 5.21.

The inverters were fabricated using the same process used for 3-terminal technology. The devices shown have the following dimensions: 4,000 x 500 x 32 nm (sources), $G_w = 1750$ nm, $D_w = 500$ nm, $g_{DS} = 20$ nm, and $g_{GS} = 50$ nm. Finally, the devices were fabricated monolithically, meaning that common gate and drain terminals were fabricated by steps 1-4, and both sources were generated at the same time by steps 5-6 of process 5.6.1. Alternatively, separately fabricated 3-terminal switches could be connected via bonding pads.

Figure 5.21: SEM images of monolithically fabricated WALD CNEMS Inverters; Designed Dimensions: (S) 4,000 x 500 x 32 nm, (D) 500 x 500 nm, (G) 1,750 x 500, gap$_{DS} = 20$ nm, gap$_{GS} = 50$ nm
Characterization of these devices was unsuccessful. It was observed that while the individual components of the devices switched as they were expected to (based on prior characterization studies of 3-terminal switches), no inverter operated as designed. Instead of producing a voltage transfer curve, IV characterization only showed 3-terminal switching or shorting at pull-in.

The devices shown in figure 5.21 have narrow drains and overlapping gate and drain electrodes because they were fabricated before the effort to correct for overlap and gate to drain shorting. After the initial study of cavitation/RIE effects on fabricated geometry was completed (section 5.7) the initial inverter design was redesigned in the same way that the 3-terminal switches were, i.e., mask files were altered to compensate for cavitation/RIE effects, and drains were widened to prevent shorting at actuation. Unlike the re-designed 3-terminal switches, testing and characterization of re-designed inverters showed no improvement in inverter behavior. IV studies still showed 3-terminal switching instead of the VTC expected for a functioning inverter.

This monotonous design/test/re-design iteration process was repeated several times. Each iteration a feature of the geometry, such as drain width, was changed, but iteration cycle the testing showed the exact same results. It became obvious that some design rule was missing, and that a fixed-fixed CNEMS inverter similar to those fabricated could not be constructed using the 3-terminal WALD switches already developed. At this point it was realized that a proper design study needed to be conducted to interrogate the design space and behavior of the 3-terminal electrostatically actuated switches used to construct a CMEMS/CNEMS inverter. The failure of these CNEMS inverters motivated the analytic modeling described in chapter 3, the completion/extension of a FEM model of 2-terminal TF electrostatically actuated switches, which resulted in the FEM/FD numerical model described in chapter 4 and the following design study.
5.8.2.2  Design study: Rectangular 3-terminal WALD NEMS Switches

To investigate the possibility that WALD CNEMS inverters failed because the pull-in voltage between the source and drain electrodes \( (V_{\text{pullin,DS}}) \) was smaller than the pull-in voltage between the source and gate electrodes \( (V_{\text{pullin,GS}}) \), and to find an experimentally elusive feasible solution, a numerical study was conducted using the MATLAB software given in Appendix F. In the following study the dependance of \( V_{\text{pullin,DS}} \) and \( V_{\text{pullin,GS}} \) on width of the drain electrode were explored. All other relevant geometric parameters, such as source length, source width, and gap heights were held constant. In this way the effect of the width of the drain on \( V_{\text{pullin,DS}} \) and \( V_{\text{pullin,GS}} \) could be isolated and explicitly studied, and the effect of the gate width implicitly studied.

For the numerical design study a theoretical WALD 3-terminal switch having dimensions: (S) 5,000 x 500 x 32 nm, \( g_{DS} = 20 \text{ nm} \), \( g_{GS} = 50 \text{ nm} \), was modeled. The results of the design study are given in figure 5.22.

5.8.2.3  Conclusions

In figure 5.22, \( V_{\text{pullin,DS}} \) and \( V_{\text{pullin,GS}} \) have been plotted as a function of drain width for the device geometry described above, and the data series fit by an exponential \( (V_{\text{pullin,GS}} \text{ Vs. gate width}) \) and power-series function \( (V_{\text{pullin,DS}} \text{ Vs. gate width}) \). It is clear from the figure that the set of points belonging to these curves remain disjoint for all realistic and fabricable drain widths. Therefore, for all realistic drain widths \( (D_{W} > 0) \) \( V_{\text{pullin,DS}} < V_{\text{pullin,GS}} \), meaning that for the logical case \( V_{in} = 0 \) both sources will be actuated. Thus it has been shown that there exists no feasible design space! In other words, it is impossible to construct a WALD CNEMS inverter whose components are fixed-fixed WALD NEMS rectangular 3-terminal switches using the developed technologies.
Figure 5.22: FEM/FD Design Study for fixed-fixed CNEMS Inverters with rectangular profiles. The theoretical design has a fixed length and width of 5 um and 500 nm, and $g_{DS}$ and $g_{GS}$ are fixed at 20 nm and 50 nm respectively. For the study the gate actuated pull-in voltages and drain actuated pull-in voltages were studied as a function of drain width. The study revealed that the two curves are disjoint for all possible designs. This means that no feasible design exists for a TF CNEMS inverter constructed from two rectangular fixed-fixed 3-terminal switches with out-of-plane functionality.

5.8.2.4 Design study: Symmetric Bow-tie 3-terminal WALD NEMS Switches

The design study proved its merit by revealing that for the feasible length scale there exists no feasible design space for the construction of WALD CNEMS inverters whose components are fixed-fixed rectangular 3-terminal switches using the technologies developed by this work. To design a working WALD CNEMS inverter the first question that should be asked and answered is: "What is the definition of the feasible design space?" A feasible design space for a CMEMS/NEMS inverter is one such that for all points in the set $V_{pullin,GS} < V_{pullin,DS}$. Therefore, any 3-terminal switch design whose gate and drain actuated pull-in voltages were members of this set should theoretically be a sufficient component for the construction of a CMEMS/NEMS inverter, because the logical case $V_{in} = 0$ would
not result in the unintentional actuation of the source biased by $V_{SS}$.

The second pertinent question is: "How can we construct a feasible design space using the developed fabrication technologies?" Because the feasible space includes all designs such that $V_{pullin,GS} < V_{pullin,DS}$, one could imagine by looking at figure 5.22 that the feasible space might be constructed by shifting either the locus of points $V_{pullin,GS}$ downward, or the locus of points $V_{pullin,DS}$ upward, such that the two sets intersect. This would result in some region to the left of the intersection corresponding to designs satisfying the necessary condition $V_{pullin,GS} < V_{pullin,DS}$.

The final question remaining to be answered is: "How can this be construction be achieved?" Because the pull-in voltage of an electrostatically actuated device is proportional to the gap height it is possible to shift the set of points $V_{pullin,DS}$ upward by increasing $g_{DS}$. However, if this approach is explored, the fabrication process will require that $g_{GS}$ also be increased. While feasible solutions may be found by this approach they will undoubtedly be limited by the fabrication technology itself. Because PMMA resist is used as a mask in the RIE step used for defining gap heights, and the resist/mask must remain thick enough such that metal deposition and lift-off post RIE is possible, there is a very real physical limit for the maximum gap height that may be fabricated using this process. Furthermore, as has been seen by characterization of cavitation/RIE effects, the minimum pattern width written by e-beam lithography is governed by the the resist thickness and RIE etch time. Thus the fabricate-able drain width is limited by it’s entrenchment depth.

The next option is to keep the $V_{pullin,DS}$ curve stationary and lower the $V_{pullin,GS}$ curve until the two curves intersect. Because the pull-in voltage of an electrostatically actuated device is inversely proportional to $A^{1/2}$ it is possible to lower $V_{pullin,GS}$ by increasing $A$, where $A$ is the overlap area between the gate and source electrodes. Thus feasible designs may be found for designs which have a large overlap area between the gate and source and a much smaller overlap area between the drain and source.

The first shape that comes to mind is that of a bow-tie. Bow-tie shaped fixed-fixed
Electromechanically actuated switches have been used in RF MEMS since the mid 1990s [78, 77, 76]. In RF MEMS switches RF power and switching speed are particularly important. Fixed-fixed bow-tie structures proved to be perfectly suited for RF switching applications. Fixed-fixed bow-tie structures are stiffer when compared to a similarly scaled fixed-fixed rectangular structures, which results in bow-tie switches having a higher switching speed. Also, because the anchors of a bow-tie structure are larger than for a rectangular structure, a much greater force, which is distributed at the anchors, can be carried by the switch. These two advantages that bow-tie structures hold over rectangular structures allowed for the development of reliable high-performance RF MEMS switches. An example of an RF MEMS switch is shown in figure 5.23.

![Cross section of an RF MEMS capacitive switch.](image)

**Figure 5.23**: A bow-tie shaped 2-terminal capacitive RF MEMS switch [78]

It is quite interesting to note that the reasons why the bow-tie structure has proven its utility in RF MEMS applications is completely different from why I have reasoned that
this shape is a feasible design for a 3-terminal WALD NEMS switch to be used to construct a WALD CNEMS inverter. In RF MEMS switching the bow-tie is shape resulted in improved switching speed, power handling, and reliability – which are all important traits for a high-quality MEMS/NEMS inverter. However, my primary interest in the design is that by using the bow-tie shape with the 3-terminal electrode layouts already explored by this research effort, the shape can deliver a large $A_{GS} : A_{DS}$ ratio, which should theoretically result in feasible 3-terminal switch designs whose gate and drain actuated pull-in voltages are such that $V_{\text{pullin,GS}} < V_{\text{pullin,DS}}$.

A design study was conducted to explore the bow-tie shape in search of a feasible set of designs using the MATLAB software given in Appendix F that is based off of the model described in chapter 4. In this study $V_{\text{pullin,GS}}, V_{\text{pullin,DS}}$ were studied as a function of drain width and the bow-tie parameter $W_M$. Figure 5.27 shows a schematic of a general bow-tie shape with bow-tie shape parameters given. To isolate the dependence of the pull-in voltages on the drain width and $W_M$, all other relevant geometry parameters were held constant.

The devices studied had the following fixed dimensions: (S) $L = 5,000\,\text{nm}$, $t = 32\,\text{nm}$, $W_o = 250\,\text{nm}$; $g_{DS} = 20\,\text{nm}$, $g_{GS} = 50\,\text{nm}$. The results of the design study are given in figure 5.25.

5.8.2.5 Conclusions

The study was successful in that a feasible design space was identified. The feasible region has been circled in figure 5.25. $V_{\text{pullin,DS}}$ and $V_{\text{pullin,GS}}$ for $W_M = \{3, 3.5\}$ um have been plotted as a function of drain width for the device geometry described above, and the data series fit by exponential functions ($V_{\text{pullin,GS}}$ Vs. gate width) and a power-series function ($V_{\text{pullin,DS}}$ Vs. Gate width). In the study the parameter $W_M$ was varied from $W_o$ to 3.5 um. The case $W_M = W_o$ is corresponds to a rectangular structure. As is seen by comparing the bow-tie and rectangular studies, figures 5.25 and 5.22, this case is identical that studied by the previous study, and has been included here to emphasize the disparity
Figure 5.24: Schematic of a bow-tie shaped structure with bow-tie parameters labeled; L := length, $D_W$ := drain width, $W_o$ := minimum half-width, $W_M$ := maximum half-width between structures.

It was observed that $V_{pullin,DS}$ is independent of the parameter $W_M$ for all designs explored. This makes sense because for all the designs studied the electrostatic load for drain actuation is distributed only over the region where $W = W_o$. Thus regardless of whatever value $W_M$ may be, for some prescribed value of $D_W$ the modeled devices have the same bending moment of inertia, which implies the same stiffness, and therefore the same pull-in voltage for equal. This was also shown analytically in chapter 3.

The effect of increasing the bow-tie parameter, i.e., changing the profile from a rectangle to a bow-tie, was to decrease the gate actuated pull-in voltage as was predicted. We see that for $W_M = 3.5$ um the locus of points corresponding to $V_{GS}$ has been lowered such that the set of points $V_{GS}$ and $V_{DS}$ (for all designs) intersect. The sets intersect for $D_W \approx 375$ nm. Thus any bow-tie shaped 3-terminal WALD NEMS switch having dimensions: $L = 5000$ nm,
Bowtie Design Study: Actuation Voltage Vs. Drain Width (Bowtie Parameter Constant)

Figure 5.25: FEM/FD Design Study for fixed-fixed CNEMS Inverters with bow-tie profiles. The theoretical design has a fixed dimensions: \( L = 5000 \text{ nm}, g_{DS} = 20 \text{ nm}, g_{GS} = 50, \) and \( W_o = 250 \text{ nm} \). For the study the gate actuated pull-in voltages and drain actuated pull-in voltages were studied as a function of drain width while the bow-tie parameter \( W_M \)

\[ W_M = 3.5 \text{ um}, W_o = 250 \text{ nm}, g_{DS} = 20 \text{ nm}, g_{GS} = 50 \text{ and } D_W < 0.375 \text{ um} \] is a feasible design satisfying the condition \( V_{pullin,GS} < V_{pullin,DS} \) required to construct a fixed-fixed WALD CNEMS inverter. Furthermore, we can conclude that any designs with dimensions residing left of the intersection are feasible 3-terminal designs.

5.8.3 Design and Fabrication of Bow-tie Shaped 3-terminal WALD NEMS Switches

Based on the characterization of cavitation/RIE processing effects and the described numerical design studies WALD NEMS bow-tie inverters/3-terminal switches with entrenched electrodes have been designed and fabricated. The bow-tie study revealed that \( D_W^* \approx 375 \)
um was the critical drain width, which means that $D_W < D^*_{W}$ to ensure $V_{pullin,GS} < V_{pullin,DS}$. Furthermore, in order to avoid the unstudied, and possibly deleterious effects of source/gate contact resistance the difference $\Delta V = V_{pullin,DS} - V_{pullin,GS}$ should be maximized if possible.

The dimensions of the fabricated bow-tie WALD NEMS devices are as follows: $L = 5000$ nm, $W_M = 3.5$ um, $W_o = 200$ nm, $g_{DS} = 15nm$, $g_{GS} = 50$ and $D_W = 300$ nm. For the fabricated devices $W_o$ was reduced from 250 to 200 nm to increase both $V_{pullin,DS}$ and $\Delta V_{pullin}$. Using the developed models these devices are expected to have the following actuation characteristics: $V_{pullin,GS} = 1.1427$ V, $V_{pullin,DS} = 1.226$ V, and therefore $\Delta V_{pullin} = 0.0833$ V, figure 6.20. Fabricated WALD NEMS bow-tie inverters/3-terminal switches are shown in figure 5.27.

![Pull-in Voltages for WALD NEMS 3-terminal Bow-tie Switches](image)

Figure 5.26: Expected pull-in voltages for fabricated WALD NEMS bow-tie 3-terminal switch: $V_{pullin,GS} = 1.1427$ V, $V_{pullin,DS} = 1.226$, and $\Delta V_{pullin} = 0.0833$

### 5.8.3.1 Fabrication Results

The fabrication of WALD NEMS bow-tie devices went well, but after release visual inspection via SEM revealed that the majority ($\approx 80\%$) of devices were fractured as is shown in figure 5.27. All of the fractured devices failed at the sharp corner (a stress concentration)
where the width of the WALD structure suddenly becomes parallel. Thin-film fabrication processes similar to those developed here, where structures are etched from thin-films deposited over the entire substrate, are known to introduce fabrication-induced tensile stresses in etch-defined structures. It is thus hypothesized that the fabrication-induced tensile stress at the corners is large enough to exceed the ultimate-tensile strength of the WALD material, thereby resulting in fracture of the structures.

5.8.4 Design of Poly-tie Shaped 3-terminal WALD NEMS Switches

If the hypothesis that the fracture observed for the fabricated WALD NEMS bow-tie devices was caused by stress concentrations is true, then failure can be avoided by simply removing, or minimizing the stress concentrations in the structure. On a macro-scale this is typically accomplished by filleting sharp corners. The same approach is taken here, but instead of defining some fillet radius for all of the corners a continuous $n^{th}$ order polynomial function is used to fit the geometric parameters $W_M$ and $W_o$. Depending on the order of
the polynomial, more fitting points can be defined to ensure that $W_M$ and $W_o$ are exactly satisfied. Because structures whose profiles are defined in this way resemble filleted bow-tie structures they have been dubbed ”poly-tie” structures.

5.8.4.1 Tensile Stress and Stress-concentration Study

Before fabricating WALD NEMS poly-tie devices an FEM study of the maximum von Mises stress in similarly scaled bow-tie and poly-tie structures under a tension was conducted using SIMULIA’s Abaqus FEA software. The goal of the study was to investigate the approximate efficacy of a poly-tie structure at reducing the maximum von Mises stress found in a bow-tie structure under tension. Because the value of tensile stress in the WALD is unknown, an arbitrary tensile load of 100 Pa was applied to the structures and the ratio of maximum stresses calculated. In this way it was possible to reach some approximate understanding of how the shape of these structures magnifies the fabrication-induced tensile stress.

The shape of the poly-tie structure was constructed by fitting the bow-tie parameters $W_M$ and $W_o$ using a $9^{th}$ order polynomial to describe the the profile of the device in the quadrant defined by $-L/2 \leq x \leq 0$ and $z > 0$. That curve was then mirrored across the two axes of symmetry defined by the x-y and y-z planes to complete the construction. In this way the shape of the similar bow-tie is preserved, with the corners replaced by smooth and continuous curves.

For the study the dimensions of the modeled bow-tie structure remained unchanged from those fabricated. The study results are shown in figures 5.28 and 5.29. Looking at figure 5.28 we see that the maximum of the von Mises stress field for a bow-tie structure under tension is at the rectangular center where the fabricated devices were observed to fracture. Furthermore, the the region of maximum stress coincides with the entire rectangular span. Comparing this to figure 5.29, we see that the induced von Mises stress field for the $9^{th}$ order poly-tie structure is markedly different. The maximum of the stress field is still found at the
beam center, but the region of maximum stress no longer coincides with the entire connecting span ($-D_W/2 \leq x \leq D_W/2$). Instead the maximum von Mises stress is concentrated along the edge of the structure coinciding with the region of maximum curvature.

Numerically speaking, for the applied load the maximum Von Mises stress in 9th order poly-tie was reduced by 35% as compare to that in the bow-tie structure. This is a significant reduction of stress achieved by simply smoothing out the corners of a feasible bow-tie geometry. Based on this stress analysis 9th order poly-tie WALD NEMS 3-terminal switches were pursued in place of bow-tie geometries as the fundamental building blocks for WALD
CNEMS logic devices.

5.8.4.2  9th Order Poly-tie Design

In order to further attenuate the stress-field in the WALD structures the poly-tie devices were designed to be slightly larger than the previously fabricated bow-tie devices. This was done by increasing length of the structure from 5 to 8 μm, and increasing the parameter $W_M$ from 3.5 to 5 μm. For this design the drain width and parameter $W_o$ remain unchanged. The increase in length and associated increase in $A_{GS}$ substantially lowers the theoretical gate and drain actuated pull-in voltages, increases $\Delta V_{pullin}$, and expands the feasible solution space, figure 5.30.

![Graph: NEMS 9th order Poly-Tie Inverter Design Study: Actuation Voltage Vs. Drain Width](image.png)

Figure 5.30: Feasible design space for a 9th order WALD NEMS poly-tie 3-terminal device with critical dimensions: $L = 8 \text{ μm}$, $W_o = 250 \text{ nm}$, $W_M = 5 \text{ μm}$

The increase in $\Delta V_{pullin}$ allowed for the gap heights to be modified; to this effect $g_{GS}$ was increased to $\approx 65 \text{ nm}$ and $g_{DS}$ decreased to $\approx 15 \text{ nm}$. Fixed-fixed electrostatically actuated MEMS/NEMS switches are known to pull-in at gap heights corresponding to $\approx 0.55\%$ of the initial gap height, thus by increasing the gap height between the gate and source the source is
ensured to make contact with the drain electrode in the so-called linear-regime. This design alteration should make operation of these devices more reliable and prevent snap thru to the gate upon actuation.

The points fit by the 9th order polynomial that defines the profile of the poly-tie devices are listed in table 6.3, and the resulting poly-tie profile is shown in figure 5.31. Using the developed models these devices are expected to have the following actuation characteristics: $V_{\text{pullin,GS}} \approx 0.38 \text{ V}$, $V_{\text{pullin,DS}} \approx 0.61 \text{ V}$, and therefore $\Delta V_{\text{pullin}} \approx 0.23 \text{ V}$, figure 6.20.

<table>
<thead>
<tr>
<th>Table 5.7: Poly-tie geometry/fitting parameters</th>
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<tbody>
<tr>
<td>$p_1$</td>
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<tr>
<td>$p_2$</td>
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<tr>
<td>$p_3$</td>
</tr>
<tr>
<td>$p_4$</td>
</tr>
<tr>
<td>$p_5$</td>
</tr>
</tbody>
</table>

Figure 5.31: Schematic of a 9th order poly-tie WALD fixed-fixed beam with critical dimensions: $L = 8 \text{ um}$, $W_o = 250 \text{ nm}$, $W_M = 5 \text{ um}$

Compared to similarly scaled bow-tie structures the feasible design space for poly-tie structures is much larger. As a result, poly-tie switches can be designed such that the
Figure 5.32: Expected pull-in voltages for designed WALD NEMS poly-tie 3-terminal switch: $V_{\text{pullin,GS}} \approx 0.38$ V, $V_{\text{pullin,DS}} \approx 6.1$, and $\Delta V_{\text{pullin}} = 0.23$ V; Modeled device dimensions: $L = 8$ um, $g_{DS} = 15$ nm, $g_{GS} = 65$ nm, $W_o = 250$ nm, $W_M = 5$ um

difference between $V_{DS}$ and $V_{GS}$ is much greater than is possible for a similarly scaled bow-tie devices, which makes them a more attractive option for the construction of complementary WALD NEMS inverters, or any other logic device that can be constructed in a similar manner. Furthermore, because the structure significantly reduces the maximum stress caused from residual stresses in the WALD film, the reliability of poly-tie devices should exceed that of bow-tie devices.
Chapter 6

Characterization of WALD NEMS Devices

6.1 Overview

The following chapter summarizes experimental results pertaining to characterization of the devices described in chapter 5. The chapter is organized into sections that focus on a specific characterization technique, and these sections are further organized by device type. Specifically, the first section summarizes the typical switching behavior of each device described by chapter 5 as characterized by IV curves. Here two different experimental setups are described and compared. The second section details the characterization of the switching speed of a 3-terminal WALD Switch described in chapter 5, section 5.7. The third section summarizes the characterization of tunneling currents measured via IV characterization of the 1\textsuperscript{st} and 2\textsuperscript{nd} generation 2-terminal WALD devices described in chapter 5, sections 5.3 and 5.5. Finally, the reliability of several types of WALD NEMS switches is reported.

6.2 IV Characterization of Switching Behavior

6.2.1 1\textsuperscript{st} Generation 2-terminal WALD NEMS Switches

The pull-in voltages of the WALD NEMS switches were characterized by the measurement of I-V curves. The measurements were performed using an HP 4145B semiconductor parameter analyzer, MC systems 8806 probe station, and custom LabView VI used to control the parameter analyzer. The IV curves were measured by sweeping a bias voltage from
0 to $V_{\text{max}}$ in 20 mV intervals and recording the current between the drain and source of the device. Here $V_{\text{max}}$ represents a value typically greater than observed actuation, which is defined by an exponential increase in measured current. For these sweeps current was limited to avoid burn-out. Similar testing techniques have been reported to characterize CNT switching behavior [226, 135, 117, 103, 61].

Pull-in characterization of two WALD bridge type devices (dimensions: 2,000 x 700 x 30 nm, $g_{GS} = 50$ nm) was accomplished using the method described above, with the current limited to 100 nA and 500 nA. The current limit was increased from 100 nA to 500 nA because it was hypothesized that devices were not making a strong contact with the actuation electrode, and therefore the current measured might in fact have been tunneling current not contact current.

The IV curve shown in figure 6.1 shows an actuated device with current limited to 500 nA. Pull-in is clearly shown where the magnitude of measured current increases by several orders over a small change of applied voltage. The resulting IV curve has the approximate shape of a square wave, which is indicative of a properly operating device (on-off, etc).

Current was ultimately limited to 100 nA because the pull-in event was still observed in generated IV curves, and the measured pull-in voltage for switching cycles limited to 100 nA was not significantly different from those with current limited to 500 nA. Figure 6.2 shows the average pull-in, and pull-out voltage for a bridge device over five cycles. The average pull-in voltage over 5 cycles for this device was found to be $\sim 5.9$ Volts, and the average pull-out voltage $\sim 3.6$ Volts. The hysteresis observed is a result of the attractive Van der Waals force between the gold electrode and WALD device. Pull-in voltage was measured 19 times between two different devices with current limited to 100 nA, and the average pull-in voltage was found to be $4.93 \pm 0.307$ Volts. This value compares favorably, within 6%, to the theoretical pull-in voltage of 5.24 Volts for a pinned-pinned device.
Figure 6.1: I-V curve for a WALD switch with current limited to 500 nA, Pull-in voltage \(\sim\) 5.4 volts

Figure 6.2: Average pull-in and pull-out I-V curves over 5 cycles for a WALD switch with current limited to 100 nA
6.2.2 2nd Generation 2-terminal WALD NEMS Switches

The pull-in voltages of the WALD NEMS switches were characterized using I-V curves to identify pull-in. The measurements were performed using an HP 4145B semiconductor parameter analyzer, MC Systems 8806 probe station, and custom LabView VI used to control the parameter analyzer. The curves were measured by sweeping an applied bias in 100 mV intervals from 0 to $V_{\text{max}}$. Here $V_{\text{max}}$ represents a value typically greater than observed actuation, which is defined by an exponential increase in measured current. For these sweeps current was limited from 500-1,000 nA to prevent burn-out. Similar testing techniques have been described in section 6.2.1.

The IV curves shown in figure 6.3 show the switching behaviors of the device in air at atmospheric pressure, figure 6.3a, and at a pressure of 30 mTorr, figure 6.3b, with different current limits. Switching behavior was tested at varying currents because lifetime testing of the devices in section 6.5 revealed consistent failure at currents greater than 500 nA. The NEMS trench devices described here experienced no failure during these tests and easily handled currents more than 1 µA. It is thought that the previous devices failed mechanically for currents greater than 500 nA, because if the device did not make full contact with the electrode, as the current level was increased so would have been the applied electrostatic load, and thus the induced stresses.

The switching behavior in air compared to vacuum differs drastically as can be seen in figures 6.3a and b. The curves measured at atmospheric pressure are parabolic in shape, while sharp steps (abrupt increases in current) are observed for curves measured in vacuum. The steps observed in the IV curves measured in vacuum resemble those seen for electrical transport in a linear chain of gold atoms [190], as well as graphene based atomic-scale switches [205]. Standley et al. suggest that the observation of conductance steps is likely indicative that the device conductance states are multiples of highly transmitting quantum channels [205]. This indicates that for our devices contact between asperities may play an important
role in device operation and performance. Finally, figures 6.3 a and b show that there is quite a difference in pull-in voltage when the device is actuated in air versus vacuum. In air the pull-in voltage ranged between 1.5 and 2 Volts throughout the range of varied current limits, but in vacuum the pull-in domain increased to ∼1.5-2.7 Volts.

Figure 6.4 shows the pull-in voltage of the device in air and vacuum (30 mTorr) with current limited to 500 nA. In this figure the difference in pull-in behavior is more apparent. In air the pull-in voltage is ∼ 1.75 Volts, and in vacuum ∼ 2.25 Volts. Of greater interest however is the shape of the curves. As seen in figure 6.3 a the IV curve in air is continuously parabolic over the domain of applied voltage, but the IV curve in vacuum begins parabolically and then displays a discontinuous exponential increase at pull-in. Also to be noted: for low-currents (<100 nA) the IV curve in vacuum is much more shallow than that of the IV curve for the same device in air.

The large range of pull-in voltages measured in air at atmospheric pressure having a median of ∼ 1.8 Volts, varies from the theoretically predicted pull-in of ∼ 3.75 Volts by ∼ 50%, if the devices are modeled having fixed-fixed boundary conditions. If we choose to model the WALD Trench NEMS devices as simply-supported, as was the case in section 5.3, and as suggested by Chang et al [38], then the theoretically predicted pull-in voltage becomes 1.67 Volts. Simply supported boundary conditions may be more appropriate for modeling of ultra-thin beams in contact mode because during deformation atoms are thought to slide past one another in the amorphous WALD structure. Using this approximation the median experimentally measured pull-in voltage is within 8% of the theoretically expected value. The average pull-in voltage for our two-terminal 50 nm generation of WALD devices was found to be 4.93 ± 0.31 Volts, which was within ∼13% of the theoretically predicted value of 4.33 Volts. The pull-in voltage of both devices is comparable to that of a similarly dimensioned CNT device [117].
Figure 6.3: IV curves in air varying current limits b) IV curves at 30 mTorr varying current limits

6.2.3 3-Terminal WALD NEMS Switches

The standard method for characterization of NMOS transistors [209, 185] was used to characterize the 3-Terminal WALD NEMS switches. Just as for two-terminal devices,
the pull-in voltages of the 3-Terminal WALD NEMS switches are characterized via measurement of IV curves. However, for a three-terminal device the pull-in voltage dependency on applied gate bias must be studied. Device characterization was accomplished using two different experimental setups. The first apparatus has been described, and the second will be introduced and described by section 6.2.5.

For 3-terminal WALD NEM switches fabricated prior to 2010, the characterization was accomplished using HP 4145B semiconductor parameter analyzer, MC Systems 8806 probe station, and a custom LabView VI used to control the parameter analyzer as previously described. IV curves were generated by linearly sweeping an applied bias between drain and source ($V_{DS}$) from 0 to 7 Volts in 100 mV intervals, while applying a constant bias between the gate and source ($V_{GS}$). Characterization was completed by generating IV curves for a set of applied gate voltages, ranging from 0 to 3.5 Volts, stepped in 0.5 Volt intervals. Current was measured between both the source and drain electrodes ($I_{DS}$), and source and gate electrodes ($I_{GS}$) to identify shorts or any possible leakage current.
Figures 6.5a-d show characterization results for the device shown in figure 5.10. In figure 6.5a, all measured data is presented. This includes $I_{DS}$ and $I_{GS}$ Vs. $V_{DS}$ for all applied $V_{GS}$. In figure 6.5b only the IV curves for even values of $V_{GS}$ are shown. Finally, in figures 6.5c-d the $I_{DS}$ and $I_{GS}$ curves are plotted separately.

Characterization of this device revealed two regions of interest. For $V_{GS} < 2$ Volts, leakage current was measured between the gate and source electrodes, as seen in figures 6.5a,b, and d. The measured leakage current, $I_{GS}$ had a maximum of $\sim 140$ nA for $V_{GS} = 0$ Volts and was observed to decrease with increasing gate bias. Furthermore, unlike $I_{DS}$, which must be limited to prevent burnout, $I_{GS}$ displayed self-limiting behavior. This is most obvious in figures 6.5a,b where $I_{GS}$ is plotted with $I_{DS}$. Finally, the pull-in voltage was observed to increase from $\sim 4.9$ to 6 Volts as $V_{GS}$ was increased from 0 to 1.5 Volts.

For $V_{GS} > 2$ Volts no leakage current was measured between the gate and source, as seen in figures 6.5a,b, and d. In this operational regime when $V_{GS}$ is increased from 2 to 3.5 Volts the pull-in voltage was observed to decrease from 4 to 3.5 Volts (as should be expected). This actuation shift is most easily seen in figure 6.5a. For this device it appears that optimal operation occurs for $V_{GS} = 3.5$ Volts, in which case there is no measurable leakage current, and the actuation voltage is a minimum.

6.2.4 Statistical Characterization of a 3-terminal WALD NEMS Switch

Because it has been observed for each generation of devices that performance varies from chip to chip, and from test to test, a statistical analysis of the switching characteristics of the 3-terminal WALD NEMS switch was necessary to draw any significant conclusions regarding device performance. The goal of the experiment is to verify that the 3-terminal WALD NEMS switch does indeed perform as a transistor and not just a two-terminal device. In other words, what we are really interested in knowing is, when the gate bias is increased does the pull-in voltage actually decrease, as we expect it to, or does the gate bias have no significant affect on the pull-in voltage?
For the experiment, one device was characterized 13 times. For each characterization \(V_{DS}\) was applied from 0 to 3.5 Volts in 50 mV intervals, \(V_{GS}\) was applied from 0 to 2 Volts in 0.25 Volt intervals, and \(I_{DS}\) was limited to 200 nA. Because the population size is less than 30 samples, a normalized distribution was assumed using Students T-distribution. Finally, a 1-way ANOVA and Tukey’s test were used to investigate the null-hypothesis that the pull-in
Figure 6.5: a) IV curves for $V_{GS}$ ranging from 0 to 3.5 Volts (stepped in 0.5 Volt intervals), showing both $I_{DS}$ and $I_{GS}$; b) IV curves for $V_{GS}$ ranging from 0 to 3 Volts (stepped in 1 Volt intervals), showing both $I_{DS}$ and $I_{GS}$; c) IV curves showing only $I_{GS}$; d) IV curves showing only $I_{DS}$ (the leakage current)

voltages for all applied $V_{GS}$ do not significantly differ.

Average IV curves for corresponding $V_{GS}$ were calculated and compared using a 1-
way ANOVA with a 95% confidence interval. Figure 6.6 shows the average IV curves for applied gate voltages of 0 and 2 Volts, and figure 6.7 shows the average pull-in voltage and associated confidence interval for each gate voltage applied. The ANOVA analysis returned a p-value of 0.0289, which is less than $\alpha = 0.05$, thus the null hypothesis was rejected, i.e., at least one of the average pull-in voltages was found to be significantly different than the others. Because the null-hypothesis was rejected, Tukeys test was required to ascertain exactly which pull-in voltages were significantly different from each other and which were not.

Results from Tukey’s test are shown graphically in figures 6.8a,b. In the plots, the Intervals highlighted in red indicate that they differ significantly from the interval of interest, highlighted in blue. It was found that the average pull-in voltages for $V_{GS} > 1.5$ Volts are significantly lower than the average pull-in voltage for $V_{GS} = 0$ Volts, figure 6.8a. However, Turkey’s test also revealed that none of the average pull-in voltages for $V_{GS} > 1.5$ Volts are significantly different from each other, figure 6.8b. In fact, most of the pull-in voltages were found to be statistically indistinguishable, e.g., if we threw out the data for $V_{GS} = 0$ Volts none of the pull-in voltages would differ, implying that application of a gate voltage had no affect on the actuation voltage.

From this analysis we can conclude that if a large enough gate voltage is applied to the device, the actuation voltage will decrease. Ideally we would expect the actuation voltage to decrease as the gate voltage increases, but our analysis has shown that this is not true for all gains in $V_{GS}$. However, we need to remember that the ANOVA and Tukey’s test are both affected by the magnitude of variance. If there is very little variance, resulting in a tight confidence interval, then the tests will be more accurate. However large variance among populations can result in an artificially high p-value, and wide confidence intervals, which can make the comparison of sample sets more ambiguous. Looking at figure 6.6, we see a noticeable jump in variance at pull-in, a result of the non-linear snap through event. Because the analyses operate on populations of extracted pull-in voltages, and these pull-
in events are difficult to accurately identify from the experimentally measured data sets, the populations have artificially high variances, and thus wide confidence intervals. If a more accurate method for identifying experimentally measured pull-in events were used, the variance should decrease, thus allowing for a more accurate statistical analysis of the dependency of actuation voltage on applied gate voltage.

**Figure 6.6: Comparison of the average IV curves for a 3-terminal WALD NEMS switch for \(V_{GS} = 0\) and 2 Volts**

### 6.2.4.1 Shorting of 3-terminal WALD NEMS Switches

As was discussed in chapter 5, IV characterization of 3-terminal WALD NEMS switches with narrow drains \((D_W = 0.5–0.7\ \text{um})\) often times showed that the gate and drain electrodes shorted at actuation. A set of IV curves showing this behavior are given in figure 6.10. These curves were measured using the HP 4145B parameter analyzer set to linearly sweep \(V_{DS}\) from 0-4 V, and vary \(V_{GS}\) from 0-1 V in 0.25 V increments each sweep. The current was limited such that \(|I_{max}| = 250\ \text{nA}\), and both \(I_{GS}\) and \(I_{DS}\) were measured as functions of \(V_{DS}\) to identify shorting.

For all characterization studies reported in this work it was common practice to check
electrode isolation by applying a potential between all combinations of electrodes and attempting to measure any drawn current. Pre-characterization the device tested here showed isolation between drain, gate, and source electrodes, but it is clear that at pull-in, $V_{DS} \approx 2.25 \text{ V}$, the gate and drain electrodes are shorted. In the figure the short is identified by the reflected IV curves, where $I_{GS}$ Vs $V_{DS}$ is exactly $I_{DS}$ Vs $V_{DS}$ reflected across the $V_{DS}$ axis.

$I_{GS}$ is the negative of $I_{DS}$ because for the HP 4145B parameter analyzer positive currents are defined as those drawn towards a probe, and negative currents are defined as those drawn from a probe. Thus, we conclude that at pull-in instead of making contact with only the drain as intended, the source snaps-through to the gate, thereby shorting the drain to the gate, figure 6.9. Because the swept voltage is applied to the drain electrode, the measured current is drawn from the gate towards the drain probe during contact, as is shown by the given set of IV curves.

### 6.2.5 3-terminal WALD NEMS Switches with Wide Drains

To eliminate drain-to-gate shorting at pull-in the 3-terminal switches were re-designed such that the drain width was increased from 0.5 to 2 um, while the gate widths were
Figure 6.8: Tukey’s comparison of average pull-in voltages for a 3-terminal WALD NEMS switch

Figure 6.9: FEM illustration of actuation induced drain-to-gate shorting of a 3-terminal WALD NEMS switch

decreased from 1.75 to 1 um; details are found in chapter 5 section 5.7. The switching
behavior of the re-designed devices was characterized using an HP 4145B parameter analyzer as has already been described. The primary goal of this characterization study was to verify that drain-to-gate shorting was indeed eliminated by increasing the drain width of the devices. To this end, the dependence of drain-actuated pull-in voltage on $V_{GS}$ was measured as before. Two different switch designs, fixed-fixed and cantilever, were fabricated and their characterization is reported here.

### 6.2.5.1 Fixed-fixed Design, figure 6.11

IV curves for a fixed-fixed 3-terminal WALD NEMS switch having dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50 nm$, $g_{DS} = 20$ nm are given in figure 6.11. The set of curves were produced by measuring $I_{DS}$ Vs. $V_{DS}$ and $I_{GS}$ Vs. $V_{DS}$ while varying $V_{GS}$ from 0 to 3 V in 1 V increments. Current was limited to 150 nA, and $I_{GS}$ and $I_{DS}$ were
measured by the gate and drain electrode probes respectively. For all $V_{GS}$ and $V_{DS}$, $I_{GS} \approx 0$ A, thus it is clear from these that shorting at pull-in between the drain and gate has been completely eliminated.

For the characterized device $V_{\text{pullin,DS}}$ ranges from 2.25-2.5 V. For all bias cases it is observed that as $V_{GS}$ is increased $V_{\text{pullin,DS}}$ decreases. This sort of behavior is expected from a 3-terminal devices because the application of a $V_{GS}$ decreases the gap height between the source and drain.

Figure 6.11: $I_{DS}$ and $I_{GS}$ Vs. $V_{DS}$ for varying $V_{GS}$; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50nm$, $g_{DS} = 20$ nm
6.2.5.2 Cantilever design, figure 6.12

IV curves for a cantilever 3-terminal WALD NEMS switch having dimensions 3,000 x 500 x 32 nm (S), $D_W = 2 \text{ um}$, $g_{GS} = 50nm$, $g_{DS} = 20 \text{ nm}$ are given in figure 6.12. The set of curves were produced by measuring $I_{DS}$ Vs. $V_{DS}$ and $I_{GS}$ Vs. $V_{DS}$ while varying $V_{GS}$ from 0 to 3 V in 1 V increments. Current was limited to 250 nA, and $I_{GS}$ and $I_{DS}$ were measured by the gate and drain electrode probes respectively. For all $V_{GS}$, $I_{GS} \approx 0 \text{ V}$ at pull-in, thus the drain-to-gate shorting phenomenon is not experienced by these devices.

One interesting difference between these devices and their fixed-fixed counterparts is that for $V_{GS} = 3 \text{ V}$ an appreciable current was measured between the gate and source for $V_{DS} < 1 \text{ V}$. Unlike shorting currents which are identified for $I_{GS} = -I_{DS}$, here $I_{DS} = 0 \text{ A}$ and $I_{GS} > 0$ which implies that the current was drawn from the grounded source to the gate. It is hypothesized that for $V_{GS} = 3V$ and $V_{DS} < 1 \text{ V}$, the deflection of the source for $0 \leq L < 1 \text{ um}$ is great enough to induce some sort of tunneling mechanism. As $V_{DS}$ increases the electric-field interaction between the drain, source, and gate may reduce the magnitude of the electric field experienced by the tunneling electrons which would diminish the current density of tunneling electrons. It makes sense that this phenomenon would not be observed by the fixed-fixed device because the gate-actuated fixed-fixed device is stiffer and therefore would not experience the same degree of deflection for $V_{GS} = 3 \text{ V}$ and $V_{DS} < 1 \text{ V}$.

For the characterized device $V_{\text{pullin},DS}$ ranges from 2.00-2.25 V. For all bias cases it is observed that as $V_{GS}$ is increased $V_{\text{pullin},DS}$ decreases, as is expected. Furthermore, the pull-in voltages for the cantilever structure are all smaller than for the fixed-fixed structure, which is to be expected because for the applied loads the effective stiffness of the cantilever structure is less than that of the fixed-fixed structure under similar loading conditions [186].
6.2.5.3 Hysteresis

Hysteresis effects for a fixed-fixed 3-terminal WALD switch having dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50nm$, $g_{DS} = 20$ nm were measured as part of the described characterization study. To study hysteresis effects $V_{DS}$ was swept forward from 0-3.5 V and then backward from 3.5-0 V, $V_{GS}$ was varied from 0-3 V in 1 V increments, the current compliance was set to 150 nA, and $I_{DS}$ was measured via the drain probe. Results from the study are given in figure 6.13.

For all bias cases shown in figures 6.13a-d $V_{\text{pullin,DS}}$ is observed to decrease with increasing $V_{GS}$ as is to be expected. For $V_{GS} = 0$ V, $V_{\text{pullout,DS}}$ was measured to be approximately 2.65 V, but for all bias cases such that $V_{GS} > 0$ the pull-out voltage was observed to decrease from 2.65 V to an approximate average constant value of $1.8 \pm 0.11$ V. It was found that for all bias cases such that $V_{GS} \neq 3$ V the difference $\Delta V = V_{\text{pullin,DS}} - V_{\text{pullout,DS}}$ remained constant with an average value of $0.766 \pm 0.065$ V. For the case $V_{GS} = 3$ V no shift was observed in $V_{\text{pullout,DS}}$, but it was seen that $\Delta V$ was reduced to approximately 0.1 V, figure 6.13d. Pull-in/out voltages as well as their differences are listed in table 6.1.

The fact that $\Delta V$ remains constant for the bias cases $V_{GS} \neq 3$ V shows that the
Figure 6.13: Measured Hysteresis of Pull-in/out Switching Behavior for a 3-terminal WALD NEMS Device; $V_{GS}$ varied from 0-3 Volts; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50nm$, $g_{DS} = 20$ nm

Table 6.1: Pull-in and pull-out voltages from IV characterization of a 3-terminal WALD NEMS bow-tie switch

<table>
<thead>
<tr>
<th>$V_{GS}$ [V]</th>
<th>Pull-in [V]</th>
<th>Pull-out [V]</th>
<th>$\Delta V$ [V]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>3.35</td>
<td>2.65</td>
<td>0.7</td>
</tr>
<tr>
<td>1.00</td>
<td>2.70</td>
<td>1.90</td>
<td>0.80</td>
</tr>
<tr>
<td>2.00</td>
<td>2.50</td>
<td>1.70</td>
<td>0.8</td>
</tr>
<tr>
<td>3.00</td>
<td>1.90</td>
<td>1.8</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Hysteresis for these cases is independent of the applied voltages $V_{DS}$ and $V_{GS}$; therefore, it is concluded that the van der Waals interaction between the gold drain electrode and WALD source is the dominant mechanism responsible for hysteresis. For the case where $V_{GS} = 3V$ it was observed that $\Delta V = 0.1$ V, which suggests that the electrostatic load induced by
the applied 3 V gate bias dominates the attractive forces induced by the van der Waals interaction. Because the pull-out voltage for this case remains unchanged from the other cases it would appear that for this particular design and bias case $V_{DS} \approx 1.8$ V is a very close to the special equilibrium point where $F_{\text{restoring}} = F_{\text{electrostatic}} = F_{\text{vdW}}$. Finally, this study reveals that not only are the pull-in voltages of 3-terminal WALD NEMS devices tunable, but to some degree so is the switching hysteresis of the devices. It is easy to imagine that WALD NEMS memory elements designed to exploit these characteristics can be constructed.

6.2.6 Gate-actuated Switching Behavior of 3-terminal WALD NEMS Switches/IV Characterization Setup Number 2

At the same time that the 3-terminal WALD NEMS switches were redesigned to correct for shorting to the gate electrode upon actuation and leakage/shorting between the gate and drain electrode, as described chapter 5.7, a new apparatus for IV characterization became available. The apparatus consists of a National Instruments USB -6229 data acquisition system (DAQ), a 10.1 MΩ resistor, micromanipulator probe station, Ithaco DL Instruments model 1211 current amplifier, and a Dell Latitude 0530 laptop computer used to control the DAQ and record data. All equipment is connected by 50 BNC cables.

For IV characterization the DAQ has been configured to provide one variable output and one constant output. The variable output is swept linearly and all sweep parameters such as step size, rate, and extents are inputs to the VI. These output voltages are applied to either the gate or drain electrodes of the 3-terminal WALD NEMS device via the probe station.

When characterizing WALD devices using the HP 4145B semiconductor parameter analyzer, it was observed that devices typically burnt out for currents larger than 1 uA. This required that a current compliance be set to avoid burnout. The only problem with this method is that it is difficult to determine from current limited IV curves whether or not the switch fully closed. Usually the current is limited at some value greater than the current
at snap-through, and it is assumed that if the snap-through event was observed then the switch must have fully closed. To limit current in this setup a resistor is placed in series with either the drain or source depending on the desired characterization. Thus, when the switch closes the voltage drop across the resistor results in some flow of current proportional to the applied voltage. Because devices previously characterized all had actuation voltages less than 5 V, a 10.1 MΩ resistor was chosen to limit current to $\approx 500$ nA. As will be seen, the use of a resistor in series with the switch output allows for improved characterization of switching behavior because once the switch is fully closed a saturation that is proportional to the resistance value is observed in the measured IV curves.

Finally the output current is converted to an output voltage by the current amplifier. The current amplifier converts the input current to a voltage proportional to the current magnitude. For example, if the order of magnitude of the input current is a uA the amplifier is set such that an input of 1 uA will result in an output of 1 V. Thus the voltage output by the current amplifier recorded by the DAQ as the output of WALD device is directly proportional to measured current. The experimental setup for IV characterization is illustrated by a circuit diagram in figure 6.14.

![Circuit diagram for experimental IV setup](image)
6.2.6.1 IV Characterization of gate-actuated 3-terminal WALD NEMS switches

IV curves for a drain and gate-actuated 3-terminal WALD NEMS device having dimensions: 4,000 x 500 x 32 nm (S), \( D_W = 2 \) um, \( g_{GS} = 50nm \), \( g_{DS} = 20 \) nm; characterized using the setup just described are given in figures 6.15 and 6.16. To characterize the drain-actuated switching behavior of the device the DAQ was set to sweep \( V_{DS} \) from 0-2.75 V, \( V_{GS} \) was held constant at 0 V, and \( I_{DS} \) was measured by placing the 10.1 MΩ resistor in series with the device source. Pull-in was observed at \( V_{DS} \approx 2.412 \) V, and pull-out at \( V_{DS} \approx 1.781 \) V. Hysteresis was observed with \( \Delta V \approx 0.631 \) V, and is consistent to the magnitude of hysteresis measured using the HP 4145B parameter analyzer setup. The measured IV curve for drain-actuated switching is shown in figure 6.15.

To characterize the gate-actuated switching behavior of the device the DAQ was set to sweep \( V_{GS} \) from 0 - 2.75 V, a constant voltage \( V_{DD} \approx 0.5 \) mV was applied to the source, and \( I_{DS} \) was measured by placing the 10.1 MΩ resistor in series with the drain electrode. The device began to pull-in at \( V_{GS} \approx 2.346 \) V, and pulled-out at \( V_{DS} \approx 1.781 \) V. As for all of the 3-terminal WALD NEMS switches appreciable hysteresis was observed with \( \Delta V \approx 0.776 \) V. The measured IV curve for drain-actuated switching is shown in figure 6.16.

6.2.7 3-terminal WALD NEMS Bow-tie Switches

IV curves for a gate-actuated 3-terminal WALD NEMS bow-tie switch (figure 6.17) characterized using the IV setup number 2 are given in figures 6.18-6.19. To characterize the gate-actuated switching behavior of the device the DAQ was set to sweep \( V_{GS} \) from 0-3 V, a constant voltage \( V_{DD} \) was applied to the source, and \( I_{DS} \) was measured by placing the 10.1 MΩ resistor in series with the drain electrode. In the figures 3 regions of interest have been highlighted. Regions shaded in green are regions of current corresponding to source-drain contact, regions shaded by blue correspond to the range of \( V_{GS} \) during source-drain contact, and regions shaded by gray correspond to the region where the device has made contact with
Figure 6.15: Drain actuated 3-terminal WALD NEMS switch; $V_{\text{pullin}} \approx 2.412$ V, $V_{\text{pullout}} \approx 1.781$ V; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50$ nm, $g_{DS} = 20$ nm.

Figure 6.16: IV curve for a gate-actuated 3-terminal WALD NEMS switch; For the characterization a voltage of 0.5 mV was applied to the drain so that a small current could be measured upon source-drain contact; $V_{\text{pullin}} \approx 2.346$ V, $V_{\text{pullout}} \approx 1.57$ V; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50$ nm, $g_{DS} = 20$ nm.

the gate electrode.

For the characterized device, IV curves were measured for varying values of $V_{DD}$. In figure 6.18a, $V_{DD} \approx 0.075$ V, and initial pull-in to the drain was observed at $V_{GS} \approx 2.121$ V. As $V_{GS}$ was increased pull-in to the gate is observed at $V_{GS} \approx 2.386$ V. Contact between the
gate and source is indicated by the linear regions highlighted in figure 6.17a. The regions shown are approximately inversely proportional to R = 10.1M, which implies strong and nearly ohmic-contact between source and drain. As \( V_{GS} \) was swept from 3-0 V, pull-out from the gate/source contact to only drain/source contact was observed for \( V_{GS} \approx 1.797 \) V, and complete pull-out was observed at \( V_{GS} \approx 1.5 \) Volts.

In figure 6.18b, \( V_{DD} = 0.1 \) V, and initial pull-in to the drain was observed at \( V_{GS} \approx 1.631 \) V. As \( V_{GS} \) was increased pull-in to the gate was observed at \( V_{GS} \approx 1.876 \) V. As \( V_{GS} \) was swept from 3-0 V, pull-out from the gate/source contact to only drain/source contact was observed for \( V_{GS} \approx 1.837 \) V, and complete pull-out was observed at \( V_{GS} \approx 1.54 \) Volts. Figure 6.18b includes an inset of the region of the IV curve corresponding to source-to-drain contact.

![Image](image.png)

**Figure 6.17:** A 3-terminal WALD NEMS bow-tie switch; Device dimensions: \( L = 5,000, W_o = 0.4 \) um, \( W_M = 3.5 \) um, \( t = 32 \) nm (S), \( D_W = 0.3 \) um, \( g_{GS} = 65nm, g_{DS} = 15 \) nm

In figure 6.19a, \( V_{DD} = 0.25 \) V, and initial pull-in to the drain was observed at \( V_{GS} \approx 1.352 \) V. As \( V_{GS} \) was increased pull-in to the gate was observed at \( V_{GS} \approx 1.5 \) V. As \( V_{GS} \) was swept from 3-0 V pull-out from the gate/source contact to only drain/source contact
was observed for $V_{GS} \approx 0.694$ V, and complete pull-out was observed at $V_{GS} \approx 0.414$ Volts. Because the current in the IV curve is dominated by pull-in to the gate electrode, an inset of the region of the IV curve corresponding to source-to-drain contact, figure 6.19a is shown.

In figure 6.19b, $V_{DD} = 1$ V, which was evidently large enough to result in pull-in to the gate electrode. In this figure pull-out behavior is observed as $V_{GS}$ is increased from $0 - 0.35$ V. The region of current highlighted by green, $V_{GS} \approx 0.35 - 2.5$V corresponds to source-to-drain contact, and again as $V_{GS}$ is further increased pull-in to the gate is again observed at $V_{GS} \approx 2.1$ V. Strangely, it is observed that as $V_{GS}$ is swept backward from 3 - 0 V it appears that pull-out of the source from the gate to drain electrode does not occur. Stranger yet, for $V_{GS} = 1 - 0$ V, instead of pulling back into the gate, as would be expected if the behavior were symmetric, the device appears to experience a nearly complete pull-out, as $I_{DS} \approx 8$ nA. This odd behavior may be due to a slight electrical contact between the electrodes and the source which could set up a response similar to a voltage divider.

**6.2.7.1 Summary of Bow-tie IV Characterization**

For all bias cases, excluding $V_{DD} = 1$ V, it was shown that for even a narrow drain, 3-terminal switching is possible without gate to drain shorting upon actuation. This was achieved by increasing the gate to source gap height, $g_{GS}$, from 50 to 65 nm while decreasing the drain to source gap height, $g_{DS}$, from 20 to 15 nm. This allows the gate-actuated source to make contact with the drain while in the linear displacement regime, thus allowing for more control over the switching phenomena. The degree of controllability can be described by the difference between $V_{GS}$ at pull-in to the drain and at pull-in to the gate.

For each bias case an obvious dependence of pull-in/out voltages on $V_{DD}$ was measured. It was observed that increasing $V_{DD}$, which causes an initial displacement of the source, had the effect of lowering all of the pull-in and pull-out voltages, with the pull-in voltages seeming to follow a power law and the pull-out voltages best fit by a polynomial. Furthermore, the pull-in voltages describing pull-in to the drain and gate follow the same trend, which implies
that the degree of controllability is roughly constant. The same is true for the pull-out voltages describing pull-out from gate-to-drain, and then complete pull-out from the drain to the open position. This kind of dependence on $V_{DD}$ is welcome news as it implies that the actuation and pull-out voltages devices can be tuned. All pull-in and pull-out voltages extracted from figures 6.18 and 6.19 have been listed in table 6.2, and pull-in/out voltages $V_s$. $V_{DD}$ for $V_{DD} = \{0.075, 0.1, 0.25\}$ plotted in figures 6.20.

The switching behavior of 3-terminal WALD NEMS bow-tie switches was successfully characterized using the setup described in section 6.2.5, and 3-terminal switching verified. Compared to similarly characterized 3-terminal WALD NEMS switches with rectangular profiles the actuation voltage of a bow-tie switch shows a stronger dependence on pre-biasing. This suggest that this device may be better suited for 3-terminal applications. Finally, it was shown that for this device the gate-actuated pull-in voltage was less than the drain-actuated pull-in voltage. This finding completes the switching characterization of this device, validates the development of the device reported in chapter 5, and verifies that the device geometry permits the fabrication of 3-terminal WALD NEMS switches as admissible components for the construction of WALD CNEMS inverters/logic devices

Table 6.2: Pull-in and pull-out voltages from IV characterization of a 3-terminal WALD NEMS bow-tie switch

<table>
<thead>
<tr>
<th>$V_{DD}$ [V]</th>
<th>Pull-in Drain [V]</th>
<th>Pull-out Drain [V]</th>
<th>Pull-in Gate [V]</th>
<th>Pull-out Gate [V]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.075</td>
<td>2.121</td>
<td>1.500</td>
<td>2.386</td>
<td>1.797</td>
</tr>
<tr>
<td>0.100</td>
<td>1.631</td>
<td>1.540</td>
<td>1.876</td>
<td>1.737</td>
</tr>
<tr>
<td>0.250</td>
<td>1.352</td>
<td>0.414</td>
<td>1.5</td>
<td>0.694</td>
</tr>
<tr>
<td>1.000</td>
<td>-</td>
<td>-</td>
<td>2.386</td>
<td>0.350, 1.797</td>
</tr>
</tbody>
</table>
6.3 Dynamic Characterization of a 3-terminal WALD Switch: Switching Speed

The apparatus used to measure the dynamic response of the device to a forcing function is shown in figure 6.21. The apparatus consists of an Agilent 33250A function/arbitrary waveform generator, micromanipulator probe station, and an Agilent DSO6012A oscilloscope. All equipment is connected by 50 Ω BNC cables. The function generator is used to apply a square wave to the device source via the probe station. The output waveform is split and input to channel 1 of the oscilloscope where it is used as a reference signal to extract the rise and fall times of the switch response as it closes and opens. The switch output is probed at the drain terminal and at input to channel 2 of the oscilloscope. The switching speed of the device is then characterized by taking the difference of the rise and fall times between the reference signal and the switch output.

The switching speed of a 3-terminal WALD switch was successfully measured using the described apparatus. The dimensions of the characterized device are as follows: 4,000 x 500 x 32 nm (S), $D_W = 0.5 \text{ um}$, $g_{GS} = 50 \text{ nm}$, $g_{DS} = 20 \text{ nm}$. Prior to dynamic characterization the switch’s pull-in voltage was identified via IV characterization by the usual methods. From IV characterization the pull-in voltage was found to be $\approx 2.814 \text{ V}$, figure 6.23. Based off of this value, the function generator was programmed to output a 150 kHz, 6 VPP square-wave impulse with a rise/fall time of 55 ns. The impulse was applied to the device and the response recorded by the Agilent DSO6012A oscilloscope. The rise and fall times of the reference signal and the switch’s response were automatically measured by the oscilloscope and are listed in table 6.3, and the reference and response signals are plotted in figure 6.22.

6.3.0.2 Discussion

The switching speed of the device tested was characterized by taking the difference of the rise and fall times of the input and output signals. As such, the switch was observed
Table 6.3: Rise/Fall Times

<table>
<thead>
<tr>
<th>Signal</th>
<th>Rise Time [ns]</th>
<th>Fall Time [ns]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference/Input</td>
<td>55</td>
<td>50</td>
</tr>
<tr>
<td>Switch Response</td>
<td>235</td>
<td>265</td>
</tr>
</tbody>
</table>

to close in 180 ns and open in 215 ns. The disparity in switching times is a direct consequence of van der Waals interaction, which has been shown to induce appreciable hysteresis in the switching behavior of the devices. Because the device was tested as a 2-terminal switch, it may not be possible to detect failure, say by welding or stiction during dynamic characterization. Therefore after dynamic testing the device’s switching behavior was again characterized via IV response. Post-dynamical IV characterization showed the switch to be un-shorted and operable; however, a large shift in actuation voltage was observed compared to the characterized pre-dynamical behavior of the device. The post-dynamical pull-on voltage was measure to be 5 V, which is an increase of nearly 100% when compared to the 2.8 Volts measured before the switching speed of the device was measured. One explanation for this behavior may be charging of the device, but that is just speculation as the phenomenon was not studied further.

The experimentally measured switching time compares well with theory. The minimum switching time, limited only by the resonant frequency of the device, is given by equation 6.1 [186]. In this equation, $V_P$ is defined as the pull-in voltage, $V_S$ is the applied voltage, and $\omega_o$ the resonant frequency in rad/s.

$$t_s = 3.67 \frac{V_P}{V_S \omega_o}$$  \hspace{1cm} (6.1)

$$\omega_o = \sqrt{\frac{k}{m}}$$  \hspace{1cm} (6.2)
\[ m = \int_V \rho(x, y, z) dV \]  

(6.3)

From the characterization of the device we know that \( V_P \) and \( V_S \) are equal to 2.814 and 3 V respectively. The resonant frequency of the device can be approximated using a 1-d model by equation 6.2, where \( k \) is the effective stiffness of the structure, and \( m \) is the mass of the structure, equation 6.3. Using equation 6.2 the resonant frequency is calculated to be \( \omega_o = 5.16 \text{ MHz} \), and using the expressions derived in 3 section 3.2 the effective stiffness has been calculated to be \( k = 1.2078 \text{ N/m} \). Hence, from equation 6.1 the resonant frequency limited switching speed is \( t_s \approx 116.3 \text{ ns} \).

From the information known about this switch, i.e. it’s actuation voltage, 116.3 ns is the minimum theoretical switching speed, and was derived neglecting damping effects. If we consider damping then a more accurate switching speed can be calculated using equations 6.9 and 6.10. The damping dependent quality factor \( Q \) is inversely proportional to the effective viscosity \( \mu_{eff} \), which is dependent on temperature and pressure. The quality factor is calculated using equations 6.4-6.8, [186].

\[
\mu = 1.2566 \times 10^{-6} \sqrt{T} \left( 1 + \frac{\beta}{T} \right)^{-1} \]  

(6.4)

Here \( \beta = 110.33 \text{ K} \), and \( T \) is temperature in K.

\[
\mu_{eff} = \frac{\mu}{1 + 9.638 K_n^{1.159}} \]  

(6.5)

Here \( K_n \) is the Knudsen number which is the ratio of the mean free path of a gas to the characteristic length scale. The Knudsen number is calculated by the following equations,

\[
K_n = \frac{\lambda}{g_o} \]  

(6.6)

Here \( g_o \) is the initial gap height of the device.
\[
= 2.6 \times 10^{-5}
\]
\[P_{\text{Torr}}\] (6.7)

\[Q = \frac{\sqrt{E \rho t^2}}{\mu (\frac{w}{2})^2}\] (6.8)

\[t_{s,1}(Q, \omega_o) = \frac{9V_P^2}{4\omega_o QV_S^2}\] (6.9)

\[t_{s,2}(Q, \omega_o) = \frac{27V_P^2}{4\omega_o QV_S^2}\] (6.10)

According to Rebeiz, equation 6.9 tends to overestimate the actual switching speed, while equation 6.10 tends to underestimate the actual switching speed. This is a consequence of assumptions made for the derivation of the expressions. Those assumptions are not discussed here, but are discussed by Rebeiz in [186]. Assuming ambient conditions, i.e., \(T = 298\) K and \(P = 760\) Torr, switching times have been calculated and are summarized along with the switching time calculated by equation 6.1, and the experimentally measured switching time in table 6.4. As stated by Rebeiz, equation 6.9 overestimates the measured switching time, while equation 6.10 underestimates the measured switching time. The mean value of the two switching times calculated by equations 6.9 and 6.10 differs from the measured switching time by only 7%, thus the actual switching time is well bound by the two approximations.

Table 6.4: Summary of theoretical and measured switching speeds

<table>
<thead>
<tr>
<th>Method</th>
<th>Time [ns]</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>180</td>
<td>–</td>
</tr>
<tr>
<td>Eq. 6.1</td>
<td>116.3</td>
<td>35.40</td>
</tr>
<tr>
<td>Eq. 6.9</td>
<td>96.5</td>
<td>46.36</td>
</tr>
<tr>
<td>Eq. 6.10</td>
<td>289.6</td>
<td>60.91</td>
</tr>
</tbody>
</table>
6.4 Characterization of Tunneling Current for WALD NEMS Devices

6.4.1 Characterization of Tunneling Current Using STM theory

6.4.1.1 1st Generation WALD 2-terminal Switches

Tunneling behavior of the 50 nm WALD NEMS two-terminal switches was investigated using the same methods described in section 6.2.1; however, the bias maximum was 2 V, and current was limited to 10 nA. Results are shown in figure 6.24a. By following scanning tunneling microscopy (STM) theory that has been previously applied to MEMS tunneling accelerometers [129, 48, 85], tunneling current is given by equation 6.11. Here $V_b = \text{bias voltage}$, $g = \text{gap height}$, $\phi = \text{effective barrier height}$, and $\alpha = 1.025 \ eV^{-1/2} \AA^{-1}$.

$$I_t \propto e^{(-\alpha \sqrt{\phi} g)}$$  \hspace{1cm} (6.11)

Following the example set by Cui et al, a semi-log plot was created of measured current versus displacement, figure 6.24b [48]. Because it was not possible to directly measure the gap height as a function of applied voltage, device displacement was instead approximated using two different methods. The first method uses a linear approximation of equation 5.3 to derive a rough closed-form solution for displacement as a function of applied voltage. In equation 6.12, the displacement has been approximated by assuming the higher-order terms of length, in equation 5.3, to be insignificant when compared to first order terms of length. As our length scales are nano this represents a justifiable linearization. In the equation $\epsilon_o$ is the permeability of free space, $A$ is the area over which the electrostatic load is distributed, $k_{eff}$ is the effective stiffness of the device, $g_o$ is the initial gap height, and $V$ the applied potential.

$$y = \sqrt{\frac{\epsilon_o A}{2k_{eff} g_o}} V$$  \hspace{1cm} (6.12)

Using equation 6.12, and the semi-log plot of measured current, the barrier height is
found to be $\phi \sim 0.0036 eV$. Hysteresis for tunneling behavior of the 50 nm WALD device was also investigated and is shown in figure 6.24c. For this limited range of operation no hysteresis was observed, implying predictable and controllable device behavior. Because tunneling current is a function of gap height only, it should remain constant for a given height, therefore sweeping voltage forward or backward should have no effect on level of measurable current, as has been shown. The data presented suggest that within a limited region (before snap-through) the WALD NEMS device may behave as a tunable tunneling device tunable in respect that the gap height and subsequently measured current can be adjusted via applied voltage.

6.4.1.2 FEM Enhanced Tunneling Characterization using STM Theory

Device displacement as a function of applied voltage has also been approximated using the 2-D multi-physics FEM model described in chapter 4 and given in appendix F. Semi-log plots were created of measured current versus displacement, figures 6.25 and 6.26, using the displacements approximated by the developed analytic and FEM models for both the 1st and 2nd generation 2-terminal WALD switches described in chapter 5, sections 5.3 and 5.5. Results are summarized in figures 6.25 and table 6.5 for the 1st generation devices, and in figures 6.26 and table 6.6 for the 2nd generation devices.

<table>
<thead>
<tr>
<th>Approximation</th>
<th>$\phi$ [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>0.0036</td>
</tr>
<tr>
<td>FEM</td>
<td>0.0069</td>
</tr>
<tr>
<td>% Difference</td>
<td>44.30 %</td>
</tr>
</tbody>
</table>

Initially, using the analytic approximation, a barrier height of $\phi \approx 0.0036 eV$ was calculated for the 1st generation devices. Using FEM approximated displacements however, an improved barrier height of 0.0069 eV has been calculated, a difference of $\approx 44.3\%$. The
Table 6.6: Work functions extracted from figure 6.26

<table>
<thead>
<tr>
<th>Approximation</th>
<th>$\phi$ [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>0.015</td>
</tr>
<tr>
<td>FEM</td>
<td>0.085</td>
</tr>
<tr>
<td>% Difference</td>
<td>82.50%</td>
</tr>
</tbody>
</table>

FEM approximation is considered to be an improvement because a barrier height of 0.0036 eV, while comparable to that reported in [85], is very low when compared to that of barrier heights for MEMS accelerometers typically reported, thus a greater value should be regarded as more accurate [48, 85, 129].

The extracted barrier height for the 2nd generation device using a linearized analytic approximation of displacement was found to be $\approx 0.015$ eV, and using the FEM approximation $\approx 0.085$ eV, a difference of $\approx 82.5\%$. These results are quite exciting for two reasons. First, the barrier height for the trench devices, extracted using the linear approximation of displacement, is an improvement over the values extracted for the first generation devices because it is of the same magnitude as barrier heights reported in literature. Second, the barrier height extracted using an FEM approximation, $\phi \approx 0.085$ eV, compares well with the reported barrier height of 0.05 eV for typical MEMS tunneling accelerometers that use Au for the anode/cathode materials, and whose electrodes have some degree of surface contamination [129].

All of the devices described in this dissertation use Au for the anode and W for the cathode; Au has a work function of $\approx 5.1$-5.47 eV, and W a work function of $\approx 4.32$-5.22 eV. Because the work functions of W and Au are similar, it was hypothesized that when operated as tunneling devices the barrier height of WALD devices would be comparable to that of the MEMS tunneling devices reported in literature [129]. The surface contaminates on the devices tested here are likely similar to those discussed by Kubena et al, e.g. organic/water, and in addition include native WO3, which is known to grow on W when WALD is
exposed to air. The results reported verify the hypothesis, and strengthen the idea that the technology developed here may eventually be used to fabricate a new class of tunable NEMS tunneling devices.

6.4.2 Characterization of Tunneling Using the Extended Field Emission Model

The tunneling current for four different WALD NEMS devices has been characterized using the extended field emission tunneling model developed by this research effort and described in chapter 3 section 3.5. The characterization was accomplished by fitting the extended field emission model to the experimentally measured IV curve for a given device. The model parameters $\phi$ and $\gamma$ of equation 3.86 were varied until a good fit was achieved. In equation 3.86 $\phi$ and $\gamma$ are the effective barrier height in eV and the number of atoms contributing to the flux of electrons respectively.

As has been discussed in chapter 3 section 3.86, device displacement as function of applied voltage must be approximated in order to apply the model to a specific electrostatically actuated device. Thus, the switching behavior for each device described was modeled using the FEM software developed here and given in appendix F. It was necessary to create "equivalent stiffness" models tailored to each specific device. This was accomplished by scaling the lateral dimensions of the FEM WALD structure until the calculated pull-in voltage exactly matched the device’s experimentally measured pull-in voltage. The use of equivalent stiffness models is necessary because experimentally measured pull-in voltages for WALD switches rarely agree with theoretically predicted values. This may be due in part to variation in fabricated dimensions, discussed in chapter 5 section 5.7, uncertainty in boundary conditions, and/or fabrication induced stresses, discussed in chapter 5 section 5.8.4. Whatever the reason may be, the measured discrepancy can be compensated by the use of equivalent stiffness models. As long as gap heights are un-scaled, the FEM approximated displacement should accurately reflect the physical displacement for corresponding to
actual and modeled applied voltage.

Using this method, the model described by equation 3.86 has been specifically used to characterize the pre-actuation tunneling current for two different 2nd generation 2-terminal WALD switches, one of which was characterized in air at atmospheric pressure and at 30 mTorr. The IV curves characterized here were given previously by figure 6.4. Both of the 2nd generation devices characterized had approximate dimensions of: 3,500 x 500 x 32 nm, \( g_o = 30 \, \text{nm} \), and their tunneling IV curves are modeled and fit in figures 6.27 and 6.28.

The third device characterized is a 3-terminal WALD NEMS switch, such as those described in chapter 5 section 5.7. The switching behavior of this particular device was characterized via IV measurements by sweeping \( V_{DS} \) and applying a constant voltage of 3 V to \( V_{GS} \). The exact IV curve characterized was given by figure 6.13 as part of the analysis of observed hysteresis in these devices. The device was measured to have the following dimensions: 4,000 x 500 x 32 nm (S), \( D_W = 2 \, \text{um} \), \( g_{GS} = 50 \, \text{nm} \), \( g_{DS} = 20 \, \text{nm} \), and it’s tunneling IV curve is modeled and fit in figure 6.29.

Finally, the fourth device characterized is a gate-actuated 3-terminal WALD NEMS bow-tie switch. The characterized device’s switching behavior has already been discussed, and the IV curve characterized here given by figure 6.18b. The IV curve that is characterized here was measured for \( V_{DD} = 0.1 \). This device had approximately the following dimensions: \( L = 5,000 \, \text{nm} \), \( W_o = 0.4 \, \text{um} \), \( W_M = 3.5 \, \text{um} \), \( t = 32 \, \text{nm} \) (S), \( D_W = 0.3 \, \text{um} \), \( g_{GS} = 65 \, \text{nm} \), \( g_{DS} = 15 \, \text{nm} \).

6.4.2.1 Discussion of Results

The parameters used for the best fit of each IV curve shown in figures 6.27-6.30 are summarized in table 6.7. As is seen by the figures, an excellent fit can be achieved using the extended field emission model, equation 3.69, specifically developed for thin-film electrostatically actuated devices. For MEMS tunneling devices having a similar material system to the devices fabricated and characterized here, barrier heights in the range of \( 0.05 \leq \phi \leq 0.055 \).
eV extracted via STM theory have been reported, with 0.55 eV approaching the theoretically expected limit for clean surfaces. For all of the devices/data fit using the extended field emission model, the barrier heights used were in the range $0.11 \leq \phi \leq 0.28$ eV, and thus are physically reasonable and in good agreement with those reported in literature [48, 85, 129, 54].

Unlike the standard model, the extended model developed by this work makes use of a second physical fitting parameter – the number of atoms. Excluding the characterization results for the 2-terminal WALD device characterized in air, only 1-2 atoms were needed to accurately fit the experimentally measured IV curves. The number of atoms used for fitting agrees well with theory, because electrons are only expected to be emitted from the point that has the highest probability of transmission. This unknown point has some physically meaningful area, thus the assumption that the point is defined by at least the cross-sectional area of one atom is reasonable.

<table>
<thead>
<tr>
<th>Figure</th>
<th>$\phi$ [eV]</th>
<th>$\gamma$ [atoms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.27</td>
<td>0.11</td>
<td>12</td>
</tr>
<tr>
<td>6.28 (30 mTorr)</td>
<td>0.15</td>
<td>1</td>
</tr>
<tr>
<td>6.28 (630 Torr)</td>
<td>0.128</td>
<td>6</td>
</tr>
<tr>
<td>6.29</td>
<td>0.24</td>
<td>1</td>
</tr>
<tr>
<td>6.30</td>
<td>0.28</td>
<td>1-2</td>
</tr>
</tbody>
</table>

In table 6.7 it is seen that the smallest lowest values of $\phi$ used for fitting correspond to the two sets of data measured in air at approximately 630 Torr (atmospheric pressure in Boulder, Colorado). Initially, the smaller values of $\phi$ suggest a more severe degree of surface contamination for these devices. However, as seen by comparing the effective barrier height of the device characterized in air at atmospheric pressure with that of the same device characterized at 30 mTorr, it is apparent that $\phi$ is not only dependent on surface conditions of the conductors but also on the environmental pressure. By decreasing pressure the average
number of molecules in the gate to source gap, as well as amount of water vapor, will also decrease. Therefore the complicated conduction path/mechanism of the free electrons is also changed, which may explain the increase in $\phi$ seen between these two devices.

Finally, in the most recently developed 3-terminal WALD NEMS devices, the minimum functional gap height ($g_{DS}$) was reduced from 30 nm to 15-20 nm. The IV curves of these devices were characterized by using larger barrier height values, $\phi = \{0.24, 0.28\}$ eV, and approximately the hypothesized minimum atomic area, $\gamma = \{1, 2\}$ atoms. The larger values of $\phi$ appear to indicate that 3-terminal devices were subject less surface contamination; however, the characterized devices were measured in the same ambient conditions as the 2-terminal devices. Furthermore, the fabrication process for these devices is much more complicated, thus one would assume that process-related surface contaminants might be more prevalent on 3-terminal devices. Therefore some other variable must be at play.

Assuming process contamination to be negligible, the primary difference between 2 and 3-terminal devices is their gap height. Using equation 6.7 the mean free path of air in Boulder at atmospheric pressure is calculated to be $\approx 40$ nm. Thus the mean free path of air at atmospheric pressure is on the same order as $g_{GS}$ of the 2-terminal devices studied, and more than 100 % greater than $g_{DS}$ for 3-terminal devices studied. Because $g_{GS} < \lambda$ there is simply less space for gas molecules to occupy, and thus the probability of molecule-molecule interaction and electron-molecule interaction is minimized. This suggests that the tunneling IV curves measured for 3-terminal devices may be more similar to IV curves measured in vacuum.

As described in chapter 3, the extended model considers electric field effects coupled with the electromechanical response of MEMS and NEMS devices. Thus, compared to the standard model which neglects electric field effects, and only considers a square potential barrier, the extended model offers less of a black box approach. Because the model can be used to approximate the entire pre-actuation tunneling IV curve, the results shown in figures 6.27-6.30 suggest that the developed model more accurately approximates the physics of
MEMS and NEMS electrostatically actuated devices. Using this characterization technique, empirical equations for $\phi$ could be derived to help better understand device physics and the potential barrier’s dependency on pressure, water vapor, gas medium, and native oxides.

### 6.4.3 % Difference Error in Characterization Introduced by a Linear Approximation

To quantify the error introduced to the extended model by linearization of the displacement as a function of applied voltage the IV curves for 2nd generation 2-terminal WALD devices shown in figures 6.27 and 6.28 were fit using the linear approximation given by equation 6.12. As is seen in figures 6.31 and 6.32 a very good fit can be achieved using this approach. The fitting parameters $\phi$ and $\gamma$ used here are listed and compared to parameters used to fit corresponding FEM approximated IV curves reported in section 6.4.2.

<table>
<thead>
<tr>
<th>Figure</th>
<th>FEM ($\phi / \gamma$)</th>
<th>Linear ($\phi / \gamma$)</th>
<th>% Diff. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.27</td>
<td>0.11/12</td>
<td>0.098/24</td>
<td>10.9/100</td>
</tr>
<tr>
<td>6.28 (30 mTorr)</td>
<td>0.15/1</td>
<td>0.14/3</td>
<td>6.667/200</td>
</tr>
<tr>
<td>6.28 (630 Torr)</td>
<td>0.128/6</td>
<td>0.12/12</td>
<td>6.25/100</td>
</tr>
</tbody>
</table>

#### 6.4.3.1 Results

Compared to FEM, % difference errors in $\phi$ are between 6 and 10 %. The most important difference between the two approximations is that, to achieve a sufficient fit using the linear approximation given by equation 6.12, the parameter $\gamma$ must be doubled. Physically this implies that the free electrons are emitted through an atomically defined area twice as large as that predicted using an FEM approximation. The idea that such a large area could contribute to the tunneling process runs contrary to the stated hypothesis that the electrons are emitted from a single point having minimum area and maximum probability of tunneling.
Regardless of this detail, the characterized parameters $\phi$ reported here are still considered to be more accurate than those extracted using the standard STM method typically cited in literature [48, 85, 129, 54], and reported in section 6.4.1.

By linearly approximating displacement as a function of applied voltage, accurate values of the work $\phi$, within 10% of FEM, may be extracted using a completely analytic model, equation 6.13. The model may also be used to approximate the entire pre-actuation tunneling IV curve, something that is not possible using the standard model. The use of a fully analytic model is of particular utility for scientists and engineers who do not have an FEM background or access to FEM software. Furthermore, the analytic model requires no costly FEM simulations and can therefore save time spent on design and analysis.

$$I = J_o \exp \left( \frac{-4\sqrt{2m_e} \phi^{3/2}}{3hq_e \Theta \left( \frac{V}{g_o - \sqrt{\frac{\epsilon_o A}{2k_{eff} g_o}} V} + 119,306V e^{-40\times10^6t} \left( g_o - \frac{\epsilon_o A}{2k_{eff} g_o} V \right)^{-(2\times10^6t+0.384)} \right)} \right) \left( \gamma \pi r_{a-}^2 \right) (6.13)$$

with the coefficient $J_o$ is explicitly given by,

$$J_o = q_e \left( \frac{16\sqrt{2\pi m_e^{3/2}}}{3h^3} \phi^{3/2} \right) \left( \frac{2q_e \phi}{m_e} \right)$$

(6.14)

6.4.4 Tunneling Conclusions

By choosing to use an FEM analysis, and thus taking into consideration the higher-order terms of the electrostatic load, a more precise approximation of displacement has been achieved, and consequently a more accurate value for the tunneling-barrier heights of the presented devices has been extracted using both the STM model and an extended field emission model developed here. Both 2 and 3-terminal WALD NEMS devices show promise for a new class of reliable and novel tunneling devices. Acquaviva et al suggest that by replacing our electrode material with a semi-conducting material the devices would behave
similarly to metal-air-insulator-semiconductor (MAIS) diodes [6, 5]. Therefore if operated in the tunneling current regime, the WALD devices would behave as mechanically-tunable tunneling NEM-MAIS diodes.

6.5 Reliability of WALD NEMS Devices

6.5.1 1st Generation 2-terminal WALD NEMS Switches

Lifetime characterization of 1st generation 2-terminal WALD NEMS switches was accomplished using an HP 4145 parameter analyzer to continuously actuate the devices. The characterized devices with 50 nm gap heights were observed to have lifetimes greater than those of the devices with 100 nm gap heights reported earlier. Characterization revealed device life-times < 300 cycles when operated with a current limit between 250-500 nA. This improvement from devices with 100 to 50 nm gap heights can be explained using FEM models, section 5.4. The devices with 50 nm gap heights experience less stress than their 100 nm counterparts during actuation, and are thus able to operate for more cycles before complete failure. However the devices still experience stresses greater than the yield stress of tungsten, which is why they continue to fail after a small number of actuation cycles.

6.5.2 2nd Generation 2-terminal WALD NEMS Switches

As with reliability characterization of 1st generation devices, lifetime characterization of 2nd generation 2-terminal WALD NEMS switches was accomplished using an HP 4145 parameter analyzer to continuously actuate the devices. The devices characterized were observed to have lifetimes much greater than 1st generation devices. Devices were observed to fail after \( \approx 40000 \) cycles with current limited to 500 nA. This improvement upon 1st generation devices can be explained using FEM models, section 5.4. These devices experience much less stress than their 1st generation counterparts during actuation due to their decreased gap heights and increased lengths, which enables them to switch for more cycles before failure.
6.5.3 3-terminal WALD NEMS Switches

The reliability of 3-terminal WALD NEMS switches was characterized using a much more sophisticated set-up than was used for 2-terminal devices. Previously device’s lifetimes were characterized via repeated IV characterization. This was a very time intensive process, and characterization of the 2nd Generation 2-terminal switches took 3 weeks! A low frequency reliability characterization apparatus was constructed in December/January 2009/2010 that allowed accurate and relatively fast reliability characterization of 3-terminal WALD NEMS switches.

6.5.3.1 Low-frequency Reliability Characterization Apparatus

The apparatus used to characterize reliability is illustrated in 6.33. The apparatus consists of a National Instruments USB -6229 data acquisition system (DAQ), a 10.1 MΩ, Agilent 33250A function/arbitrary waveform generator, micromanipulator probe station, Stanford Research Systems SR830 DSP lock-in amplifier, and an Dell Latitude 0530 laptop computer used to control the DAQ and record data. All equipment is connected by 50 Ω BNC cables.

The DAQ is set using a LabView VI to output a constant bias $V_{DD}$ to the switch source so that a constant current output can be measured when the switch closes. A triangular waveform of frequency $\omega_{\Delta,GS}$ and amplitude $V_{\Delta,GS}$ is output by the Agilent 33250A function generator and applied at the gate terminal. As was done for IV characterization, a resistor is placed in series with the device drain to prevent burnout while the switch is closed. The current induced by the voltage drop across the resistor is input to the SR830 DSP lock-in amplifier where it is compared to an internal sinusoidal reference source that has been programmed to have a frequency $\omega_{\text{lockin}}$ and amplitude $V_{\text{lockin}}$. The lock-in amplifier is set for low-current input, and if $\omega_{\Delta,GS} = \omega_{\text{lockin}}$, outputs a constant voltage directly proportional to the RMS current to the DAQ. The output of the lock-in amplifier is recorded as a function
of time by the VI.

The output frequency of a working switch should be identical to the driving frequency $\omega_{GS}$, thus if the frequency of the internal source of the lock-in amplifier is set such that $\omega_{lockin} = \omega_{\Delta,GS}$ the output of lock-in is expected to be constant voltage for the lifetime of the switch. Hence, for a 3-terminal switch, failure can be identified by a drop or change in the output of the lock-in amplifier. As will be shown, the setup works equally well for 2-terminal testing; however, failure can only be identified for a broken or burnt-out device. If a 2-terminal device fails due to stiction, depending on the quality of contact between the source and gate electrodes, failure will not be obvious. This is untrue for 3-terminal switches because $V_{DD} \neq V_{GS}$, therefore if the device were to fail because of stiction to the gate the output current would change, and this sudden change would be reflected in the output of lock-in amplifier. Thus during 2-terminal reliability characterization it is necessary to intermittently inspect the switching behavior of the device via IV characterization.

### 6.5.3.2 Results

Using the apparatus described, the reliability of a 3-terminal WALD NEMS switch was successfully characterized. The dimensions of the devices tested are as follows: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50nm$, $g_{DS} = 20$ nm. To test the apparatus, a device whose gate and drain electrodes were shorted was characterized as a 2-terminal device. A 5 kHz triangular-wave forcing function with $V_{\Delta,GS} = 3.5 \ V_{PP}$ was applied to the source electrode using the function generator, and 0 V applied to the gate and drain-terminals via the DAQ. A 10.1 M$\Omega$ resistor was placed in series with the drain, and the parameters of the lock-in amplifier’s internal source were set such that $\omega_{lockin} = 5$ kHz and $V_{lockin} = 1$ V. Pertinent scaling and filtering settings of the lock-in amplifier used for reliability characterization are given in table 6.9. Lock-in output versus time for this characterization is plotted in figure 6.34a.

The reliability of a fully-functioning 3-terminal device was characterized by using the
exact setup illustrated by 6.33 and described above. A 500 Hz triangular wave forcing function with $V_{\Delta,GS} = 4.5 \text{ V}_{pp}$ to the source via the function generator and $V_{DD} = 0.5 \text{ mV}$ was applied to the source via the DAQ. A 10.1 MΩ resistor was placed in series with the drain, and the parameters of the lock-in amplifier’s internal source were set such that $\omega_{\text{lockin}} = 500 \text{ Hz}$ and $V_{\text{lockin}} = 1 \text{ V}$. Pertinent scaling and filtering settings of the lock-in amplifier used for reliability characterization are given in table 6.9. Lock-in output versus time for this characterization is plotted in figure 6.34b.

Table 6.9: Lock-in Amplifier settings for reliability characterization of WALD NEMS devices

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>$1 \times 10^6$</td>
</tr>
<tr>
<td>Slope/oct</td>
<td>24 db</td>
</tr>
<tr>
<td>Sensitivity</td>
<td>1x1 uA</td>
</tr>
<tr>
<td>Reserve</td>
<td>normal</td>
</tr>
<tr>
<td>Filters</td>
<td>line</td>
</tr>
</tbody>
</table>

6.5.3.3 Results

Characterization of the two devices using the described apparatus was successful. The drain-actuated switch was observed to operate for more than 11 M cycles, figure 6.34a, and the gate-actuated switch was observed to operate for $\approx 2.14 \text{ M cycles}$, 6.34b. Failure of the gate-actuated device is identified in figure 6.34b where the lock-in output drops suddenly from $\approx 11 \text{ nA}$ to $\approx 8.5 \text{ nA}$. Failure of the drain actuated switch is not observed in 6.34a. The drop in current is because the experiment was stopped to test for possible failure due to stiction via an IV sweep. Post-reliability IV characterization showed the device to be in working order so reliability characterization was continued. No failure was observed in the second reliability test, however, post-reliability IV characterization revealed that the device had failed via stiction at some point during the second reliability test. For this reason only the number of cycles recorded during the first test are reported here.
Without a sufficiently sized sample set no statistically meaningful conclusions can be stated in regards to the characteristic reliability of these devices. However, we can say that it appears that the tested 3-terminal WALD switches have lifetimes on the order of $10^6$ cycles, and that device reliability may be dependent on actuation method and electrode geometry. It may be possible to explain the apparent dependence of device reliability on both actuation method and electrode geometry, by considering the effective stiffness of the device under each loading case.

Applying the expressions derived in chapter 3 section 3.2 to the device and loading cases studied here, the effective stiffness of the drain-actuated device is calculated to be $\approx 2.02 \text{ N/m}$, and the effective stiffness of the gate-actuated device is calculated to be $\approx 8.73 \text{ kN}$. Therefore we see that for these devices the effective stiffness of the WALD structure subject to a gate-distributed load is over 4 times greater than when subject to a centrally located drain-distributed load. Not only does this imply a large difference in pull-in voltages between the two actuation methods, but it implies that a larger force must be applied in order to achieve the same displacement required for actuation. A larger force implies greater stresses, and greater stresses over millions of cycles should be expected to result in shorter lifetime. In the future this should be studied statistically by varying the width of the gate and drain electrodes and testing the devices using the apparatus described.

### 6.5.4 Reliability of 1st Generation WALD NEMS Tunneling Devices

The experimental procedure used for pull-in characterization was modified to accommodate lifetime testing for tunneling operation. Current was limited to 20 nA and actuation voltage was switched directly from 0 Volts to a value large enough to induce electron tunneling. A LabView VI code was written to record one sweep for every one hundred cycles. After several thousand cycles tunneling behavior was examined via an IV curve to ensure the device had not failed. Using this method we have demonstrated that our two-terminal tunable NEMS WALD tunneling device has a lifetime greater than 660,500 cycles, figure 6.35.
FEM models show maximum Von Mises stresses less than tungsten's yield stress for displacements experienced by the mechanical structure of the device during operation. Therefore mechanical failure of the device should not be expected.

6.5.5 Reliability of 2nd Generation 2-Terminal WALD NEMS Tunneling Devices

The tunneling-lifetime test was modified for testing the WALD entrenched devices because of the large amount of time required to conduct the test using a parameter analyzer. The WALD entrenched devices were actuated by a 300 Hz sine wave with an amplitude of 0.5 Volts and a DC offset of 1 Volt. After several hours the device's IV curve was measured using the parameter analyzer to check for failure and to decide if the device was still working properly.

The WALD entrenched devices have been successfully actuated more than $5 \times 10^6$ cycles without failure. IV curves revealed that during testing the actuation voltage for low-current operation had drifted slightly from $\sim 1$ volt to 1.5 Volts, but no drastic difference in pull-in voltage was observed for contact switching. This increase in low-current actuation voltage may be due to strain hardening, or possibly to some degree of charge trapping.
Figure 6.18: IV curve for gate-actuated switching of a 3-terminal WALD NEMS bow-tie switch; $V_{DD}$ is varied as 0.075, 0.1 V in figures a, b respectively; In the figures regions shaded in green are regions of current corresponding to source-drain contact, regions shaded by blue correspond to the range of $V_{GS}$ during source-drain contact, and regions shaded by gray correspond to the region where the device has made contact with the gate electrode; In figure (a) after pull-in to the gate several saturation regions whose slopes are inversely proportional to $R = 10.1 \, \text{M} \Omega$ are highlighted by dashed lines.
Figure 6.19: IV curve for gate-actuated switching of a 3-terminal WALD NEMS bow-tie switch; $V_{DD}$ is varied as 0.25 and 1 V in figures a and b respectively; In the figures regions shaded in green are regions of current corresponding to source-drain contact, regions shaded by blue correspond to the range of $V_{GS}$ during source-drain contact, and regions shaded by gray correspond to the region where the device has made contact with the gate electrode.
Figure 6.20: Pull-in/out voltage Vs. $V_{DD}$ for the 3-terminal WALD NEMS bow-tie switch shown in 6.17 characterized in figures 6.18 and 6.19

Figure 6.21: Circuit diagram for experimental impulse response setup; The response of the device to a square wave is used to characterize switching speed
Figure 6.22: Square wave response of a drain-actuated 3-terminal WALD NEMS switch, the reference signal is plotted in green, and the switch response in blue; From this plot rise and fall times of 180 and 210 ns were calculated; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 0.5$ um, $g_{GS} = 50$ nm, $g_{DS} = 20$ nm

Figure 6.23: Measured IV curves taken before and after the impulse response experiment; Before the test $V_{pullin} = 2.814$V, and after the test this value shifted to $V_{pullin} = 5$ V; Device dimensions: 4,000 x 500 x 32 nm (S), $D_W = 2$ um, $g_{GS} = 50$ nm, $g_{DS} = 20$ nm
Figure 6.24: a) Low current I-V. b) Log(Current) Vs. displacement, $\phi \sim 0.0036eV$. c) Hysteresis analysis of tunneling current
Figure 6.25: Semi-log plot of tunneling current for a 1st generation fixed-fixed 2-terminal WALD device; Device dimensions: 2000 x 700 x 32 nm, gap ~ 50 nm

Figure 6.26: Comparison of extracted barrier heights using linear and FEM approximated displacements for a 2nd generation 2-terminal WALD device; Device dimensions: 3000 x 500 x 32 nm, gap ~30 nm
Figure 6.27: Extended tunneling model fit to the IV curve of a fixed-fixed 2nd generation 2-terminal WALD switch; Device dimensions: 3,500 x 500 x 32 nm (S), $g_{GS} \approx 30$ nm; Fitting parameters: $\phi = 0.11$ ev, $\gamma = 12$ atoms

Figure 6.28: Extended tunneling model fit to the IV curves of a 2nd generation 2-terminal WALD switch taken at 1 atm and 30 mTorr; Device dimensions: 3,500 x 500 x 32 nm (S), $g_{GS} \approx 30$ nm; Fitting parameters: $\phi = 0.128$ ev, $\gamma = 6$ atoms (1 atm), and $\phi = 0.15$ ev, $\gamma = 1$ atom (30 mTorr)
Figure 6.29: Extended tunneling model fit to the IV curve of a fixed-fixed 3-terminal WALD switch; Device dimensions: 4,000 x 500 x 32 nm (S), $G_W = 1,000$ nm, $D_W = 2,000$ nm, $g_{GS} \approx 50$ nm, $g_{DS} \approx 50$ nm; Device was drain actuated with $V_{GS} = 3$ V; Fitting parameters: $\phi = 0.24$ ev, $\gamma = 1$ atoms
Figure 6.30: Extended tunneling model fit to the IV curve of a fixed-fixed 3-terminal WALD bow-tie switch; Device dimensions: \( L = 5,000 \) nm, \( W_o = 0.4 \) um, \( W_M = 3.5 \) um, \( t = 32 \) nm (S), \( D_W = 0.3 \) um, \( g_{GS} = 65nm \), \( g_{DS} = 15 \) nm; Device was gate actuated with \( V_{DD} = 0.1 \) V; Fitting parameters: \( \phi = 0.28 \) ev, \( \gamma = 1 - 2 \) atoms
Figure 6.31: Extended tunneling model fit to the IV curve of a fixed-fixed 2nd generation 2-terminal WALD switch via equation 6.12; Device dimensions: 3,500 x 500 x 32 nm (S), $g_{GS} \approx 30$ nm; Fitting parameters: $\phi = 0.11$ ev, $\gamma = 12$ atoms

Figure 6.32: Extended tunneling model fit to the IV curves of a 2nd generation 2-terminal WALD switch taken at 1 atm and 30 mTorr via equation 6.12; Device dimensions: 3,500 x 500 x 32 nm (S), $g_{GS} \approx 30$ nm; Fitting parameters: $\phi = 0.128$ ev, $\gamma = 6$ atoms (1 atm), and $\phi = 0.15$ ev, $\gamma = 1$ atom (30 mTorr)
Figure 6.33: Circuit diagram for low-frequency reliability characterization experimental setup
Figure 6.34: Reliability characterization of a gate and drain-actuated 3-terminal WALD NEMS switch; (a) Device was drain-actuated for \( \approx 11 \) M cycles before failure; (b) Device was gate-actuated for \( \approx 2.138 \) M cycles before failure; Device dimensions: 4,000 x 500 x 32 nm (S), \( D_W = 2 \) um, \( g_{GS} = 50 \) nm, \( g_{DS} = 20 \) nm
Figure 6.35: IV curve of lifetime testing for a doubly clamped device shown to have a lifetime > 660,500 cycles. Plot shows 3 sweeps at different cycle numbers during the lifetime testing of the NEMS WALD tunneling device.
Chapter 7

Conclusions/ Future Work

7.1 Dissertation Summary

The primary focus of the research reported in this dissertation was the development of CMOS compatible atomic layer deposition (ALD) enabled NEMS switches suitable for high temperature and or high-radiation environments. As chapters 5 and 6 attest, a great deal of work has gone into the development of a novel, low-temperature, top-down, CMOS compatible, ALD nano-fabrication process for the development of multi-terminal, electrostatically actuated NEMS switches and logic devices. The process developed is both an extension of established micro-surface machining processes, and a unique contribution to state-of-the-art NEMS thin-film fabrication techniques. The process has been developed over many generations of devices: from the 1st generation devices, whose design was similar to more traditional MEMS designs [54], to the more creative and novel 3-terminal designs, which include multiple entrenched electrodes and symmetric non-rectangular WALD structures. These later devices have been designed as the fundamental building blocks for thin-film WALD NEMS logic devices, which could be extended to all mechanical computing architectures.

Besides introducing novel top-down surface micro-machining techniques, the processes used WALD as a structural material for the first time [54, 52, 195]. The devices fabricated to date show that WALD, and for that matter any ALD thin-film, is suitable for use in future NEMS devices. In fact, ALD thin-films are more than suitable when compared to their CVD counterparts. They are superior because of their conformal coating, controllability, and low-
temperature deposition [195, 194, 63, 83, 82, 121, 137, 193, 227]. Additionally, the process developed should be compatible with any planar thin-film material for the fabrication of NEMS devices and should consistently produce a much higher yield of devices per chip when compared to CNT processes [61, 102, 103, 135], or to more recent state of the art thin-film processes [105, 51].

The developed WALD NEMS process has proven itself more than capable of meeting future design requirements in the development of NEMS devices competitive with state-of-the-art technologies [51, 102, 140, 174, 204, 236]. The 2-terminal entrenched WALD switches first reported in [52] compare well to, or outperform, similar CNT devices [9, 61, 102, 103, 117, 119, 135, 226], state-of-the-art graphene devices [140, 204], and MEMS tunneling devices [48, 85, 129]. The 3-terminal WALD devices outperform their nearest CNT counterparts [102, 135] and represent a completely unique thin-film NEMS device as far as geometry, scale, gap heights, and design are concerned. When considering actuation voltage, the 3-terminal WALD switches presented in section 5.6 outperform their nearest competitors by 3-10 volts [105, 51, 104, 102, 135, 236]. Finally, inverters constructed from 3-terminal WALD NEMS bow-tie or poly-tie switches would represent the state-of-the-art in thin film mechanical logic technology.

Though the primary goal of this research was the development of CMOS compatible ALD tungsten thin-film devices suitable for use in high-temperature and/or high radiation environments, the pursuit of this goal resulted in many other notable accomplishments in analytic and computational modeling. The analytic models developed in chapter 3 greatly extend the design tools available to the engineer. The derived pull-in models for electrostatically actuated thin-film switches with symmetric and non-rectangular profiles offer a fast and efficient method for the design of complicated MEMS or NEMS 2/3-terminal devices that could easily be extended to n-terminal designs. These models could also be implemented as cost functions for cheap optimization studies.

The van der Waals analysis conducted in chapter 3 sheds light on the system dynamics
for a complicated non-linear system, with an emphasis on the understanding of system stability. This work led to the derivation of detachment curves that were later used in chapter 4 to help verify more accurate FEM generated detachment curves. Also in chapter 3, the standard Fowler-Nordheim model was extended to include the electromechanical response of a thin-film NEMS switch in order to better characterize measured pre-actuation currents. The model is a significant step forward from STM models previously used in the field to characterize MEMS and NEMS tunneling devices.

Finally, large contributions and gains have been made through use of the developed multi-physics FEM model. A faux-Lagrangian finite difference scheme was developed to solve Laplace’s equation in a deformable electrostatic domain having height-to-length ratios on the order of $10^{-3}$. The solver allows the numerical study of NEMS devices having extremely small functional gap heights. For this reason the method is seen as an improvement over boundary element methods commonly used by commercial software to solve electromechanical problems which have been observed to diverge for such domains. Furthermore, complicated and extensive design studies can easily be conducted using developed software given in appendix F. Using this model, design rules specific to thin-film NEMS inverters constructed from 3-terminal fixed-fixed thin-film switches were discovered, which led to the development of bow-tie and poly-tie geometries. It was shown that device displacements approximated using the multi-physics model were much more accurate than those calculated using derived analytic approximations, which allowed for much more accurate tunneling characterization of WALD NEMS devices using both the standard STM model and the extended field-emission model developed here.

7.1.1 List of Major Achievements

Major achievements are listed as follows:
1. During the course of this research two different novel, top-down, low-temperature, CMOS integrable fabrication technologies, employing WALD as a structural layer for MEMS or NEMS devices, were developed. The fabrication processes developed are robust yet simple, and are capable of producing a wide array of novel NEMS devices. The developed fabrication processes build upon traditional micro-machining techniques and introduce new methods specifically suited for NEMS thin-film devices, thereby expanding the possibility of future fabrication technologies and associated devices.

2. Using the developed fabrication technologies several generations of WALD NEMS switches were successfully designed, fabricated, and characterized. Previously, ALD materials had been used primarily as protective coatings, or hydrophilic/hydrophobic coatings, but here, for the first time an ALD material was successfully integrated into a nano-scale fabrication process as the structural material for an electrostatically actuated device. The ultra-thin films allowed for the fabrication of devices with very low, CMOS compatible actuation voltages. Characterization of the WALD switches developed here demonstrated functionality in a low-current tunneling regime. Thus the devices have the potential to be used as the building blocks for novel devices not possible using traditional CMOS technology, i.e., high-density tunneling logic devices.

Demonstrated WALD NEMS switches include:

* 2-terminal, surface micromachined WALD NEMS fixed-fixed and cantilever switches having gate-to-source gap heights of 50 nm
* 2-terminal, entrenched WALD NEMS fixed-fixed switches having gate-to-source gap heights of 30 nm
* 3-terminal, entrenched WALD NEMS fixed-fixed and cantilever switches having gate-to-source gap heights of 50-65 nm, and drain-to-source gap heights of 20
nm

* 3-terminal, entrenched WALD NEMS fixed-fixed bow-tie and 9th order poly-tie switches having gate-to-source gap heights of 50-65 nm, and gate-to-source gap heights of 20 nm

3. A FEM/FD based multi-physics model for 2 or 3-terminal devices whose electrostatic domain has an aspect ratio on the order of 10^{-3} was developed. The model uses a faux-Lagrangian mesh finite difference method to solve the Potential problem (Laplace’s Equation) for a quasi-statically deforming domain. The approach developed here allows for the study, and numerical characterization, of thin-film NEMS device designs which are not feasible using a commercially typical non-specialized FEM/BEM approach. Using the FEM/FD based numerical model, coupled with the extended tunneling model, the characterization of the tunneling regime has been improved. Furthermore, the development of this model allowed for the discovery of CNEMS Inverter design rules specific to ultra-thin film NEMS devices similar to those developed by this research effort.

7.2 **Envisioned Future Work**

7.2.1 **Devices**

This work only begins to explore the types of device that could be fabricated using WALD. Using e-beam, or FIB, extremely small devices with very high resonant frequencies could be fabricated. Depending on quality factors, ultra-sensitive ALD NEMS resonant sensors for use in harsh environments could be developed. The possible functionalization of potential ALD NEMS resonators for use in various bio-sensing applications could also be studied as part of this potential project.

In chapter 6 it was seen that 3-terminal WALD devices with wide drain electrodes experienced predictable hysteresis for multiple biasing conditions which was attributed to
van der Waals interactions. This behavior could be studied in depth through use of AFM and
the models developed here to garner a thorough understanding of the interaction. This study
would allow for the design and development of CMOS compatible WALD NEMS memory
elements.

Lastly, the development of WALD NEMS logic devices should be continued. Building
from the work of this thesis, all of the necessary design tools have been developed, thus
the fabrication of working devices should feasible assuming the availability of sufficient fab-
rication tools/facilities. In parallel with the development of these devices should be the
development of IC/NEMS hybrid systems. This may begin with the demonstration of a
simple resistive inverter constructed by one 3-terminal NEMS switch and a doped silicon
resistor. The development of WALD NEMS logic devices would necessarily invoke the de-
velopment of computing architectures for controllers and processors capable of operation in
harsh environments.

Envisioned future work for the continued development of ALD enabled NEMS devices
is summarized as follows:

• Development of ALD NEMS resonant sensors for harsh environments (possible func-
tionalization?)

• Development of ALD NEMS memory elements

• Continued development of ALD NEMS logic devices

• Development of hybrid MOS IC/ NEMS ALD technologies

• Development of an ALD NEMS computing architecture

• Development and demonstration of an ALD NEMS micro-controller/ micro-processor

• Possible exploration of nano-laminate ALD materials
7.2.2 Thermal Characterization of WALD Devices

Although tungsten has the highest melting temperature of any metal, there are several possible failure mechanisms that may arise at moderately high temperatures \((T > 200^\circ C)\), which warrant thorough investigation. Several studies should be conducted to assess the reliability and performance of WALD NEMS devices in high-temperature environments. These tests entail high-temperature annealing and ambient-temperature IV/lifetime testing to investigate any possible influence of grain growth and oxidation on device performance. The switching performance of the devices should be characterized in the normal manner, but at elevated temperatures to identify any temperature-dependent shifts in actuation voltage, increases in tunneling current, or any possible failure mechanisms related to temperature-enhanced electro-migration. Finally, operationally induced oxidation, decreased conductivity of the metal, and mechanical softening of the structures, resulting from the high-temperature environment, may have a deleterious impact on device performance; therefore, switching dynamics as well as reliability should also be studied at elevated temperatures \((T > 300^\circ C)\).

7.2.3 WALD Material

Because WALD has been used here as a structural material for the first time, and the focus of the research was device development, little is known about its mechanical properties. To date bulk assumptions have been made for all modeling/design purposes. The success of future projects maybe greatly aided by improved understanding of the material properties of WALD. Intelligent design of the proposed devices, including the ability to develop accurate modeling tools, as well as garner a fundamental understanding of both theoretically and experimentally expected device behavior, relies heavily on the characterization of the material’s stiffness, residual stress, thermal expansion coefficient, and Van der Waals interaction with substrate materials. Envisioned contributions to the field of thin-film material science are as follows:
• Characterization of Young's modulus and Vicker's hardness

• Characterization of thin film residual stress and associated through-thickness stress gradient for multiple processing temperatures

• Characterization of ALD W thermal expansion coefficient (TEC)

• Characterization of surface energy interaction of both ALD W/Au and ALD W/ALD W systems, and associated Haymaker constants

• Study of thin-film grain growth mechanisms

• Study of surface energy dependency/induced thin-film tensile stress on etch technique

7.2.4 Device Physics

The actual conduction mechanism of free electrons across the functional gap of characterized NEMS devices is unknown. It has been surmised in literature, but not studied explicitly, that the mechanism is appreciably affected by surface contaminants, such as: water vapor, native oxide, and organic particles, as well as environmental parameters such as gas, pressure, and temperature. The developed model does not attempt to capture the physics of the exact conduction mechanism, instead it essentially lumps all of the unknowns into the fitting parameter $\phi$.

In chapter 6 it was shown using the tunneling model developed in chapter 3 that the characterized effective barrier height $\phi$ displays a dependency on pressure. It is thus hypothesized that the extended field emission model could be used to empirically study the dependency of the effective barrier height on various surface contaminants. This could easily be accomplished using 2-terminal WALD NEMS devices, or similar devices fabricated using different source/gate material systems, by testing the devices over a range of pressures and for an assortment of gasses. Data would then be fit using the model, and the dependency of $\phi$
on the experimental variables empirically derived. In the same way the effects of oxide could be studied in a controlled manner by depositing oxides via ALD on fabricated structures.

This work would improve the understanding of device physics at the nano-scale, thereby expanding our understanding of fundamental device limitations. An improved model would also find use as a design tool for the development of future NEMS device and packaging technologies. Furthermore, an improved understanding of the phenomena could allow for the development of completely novel tunneling devices, as well as devices optimized for minimum power consumption.

7.2.5 Computational

The FEM model developed for this research is quite limited. The current model is only capable of simulating 3-terminal devices, and as coded the inclusion of more terminals should prove to be quite troublesome. For this reason I believe that boundary element methods are ultimately best if one hopes to develop a general software package. For domains with aspect ratios > $10^{-3}$ boundary element methods excel in the handling of general domains, i.e., $n$-terminal and non-rectangular, but new and advanced methods must be developed for ultra-low aspect ratio domains. The development of these methods would prove quite rewarding and be of great use to the NEMS community.

There are several improvements that can be made to the developed model/software developed here to make it more robust. In the sake of brevity, the model could be improved in the following ways:

- An option to include internal stresses should be added
- A more efficient method for including multiple terminals in the electrostatic domain should be developed
- Non-rectangular boundaries should be considered
• Mechanical boundary conditions of variable stiffness should be included, i.e., the option to model the device as partially fixed.

• Contact mechanics should be included, this way stiction, release, and complete inverter operation could be simulated.

• The developed model should be extended to 3-dimensions. The current model is limited in its ability to study the electrostatic behavior of devices with non-symmetric profiles.

• A Casimir module should be written.

• For speed the model should be programmed in C.

If the developed software were extended as described by this "wish list", one would have an extremely sophisticated and robust model capable of accurately simulating a large variety of devices and physical phenomena. The continued development of this model would greatly aid the development and design of future thin-film NEMS devices for academic and industry endeavors.

Finally, a numerical optimization study should be conducted using the developed software. As is, the software could be used to optimize the design of 3-terminal thin-film NEMS switches and inverters. The program could be used with a Kriging interpolation to minimize pull-in voltage while maximizing the switching speed of 3-terminal devices. For inverters the program could be used to optimize the shape of 3-terminal components of a complementary NEMS inverter so that the difference between gate and drain-actuated pull-in voltages was maximized. Designs could then be verified via fabrication and characterization. If extended models of van der Waals interaction and tunneling current were available, the model could also be used to find optimal designs that minimize the tunneling current, and either maximize or minimize the pull-out voltage, depending on intended application, i.e., for memory elements or logic devices.
Bibliography


[99] Intel. A 32nm logic technology featuring 2nd-generation high-k + metal-gate transistors, enhanced channel strain and 0.171um2 sram cell size in a 291mb arra. Sep 2008.


Appendix A

List of Symbols and Abbreviations
Table A.1: List of symbols and abbreviations (A-E)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
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<tr>
<td>a</td>
<td>(m/s^2)</td>
<td>acceleration</td>
</tr>
<tr>
<td>(A_{i3j})</td>
<td>(J)</td>
<td>Hamaker constant for material (i) interacting with material (j) through medium 3</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>–</td>
<td>commonly used parameter</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>(1/\sqrt{eV\AA})</td>
<td>STM tunneling coefficient</td>
</tr>
<tr>
<td>(\alpha^*)</td>
<td>–</td>
<td>critical detachment parameter</td>
</tr>
<tr>
<td>(B)</td>
<td>–</td>
<td>differential operator</td>
</tr>
<tr>
<td>(B)</td>
<td>T</td>
<td>magnetic field</td>
</tr>
<tr>
<td>(\beta)</td>
<td>–</td>
<td>commonly used parameter</td>
</tr>
<tr>
<td>(C_{el}^i)</td>
<td>(F)</td>
<td>(i)-th elemental capacitance</td>
</tr>
<tr>
<td>(C_{tot})</td>
<td>(F)</td>
<td>total capacitance</td>
</tr>
<tr>
<td>(D)</td>
<td>–</td>
<td>drain electrode</td>
</tr>
<tr>
<td>(D_W)</td>
<td>(m, , \text{um})</td>
<td>drain width</td>
</tr>
<tr>
<td>(D)</td>
<td>Pa</td>
<td>constitutive matrix</td>
</tr>
<tr>
<td>(\Delta)</td>
<td>–</td>
<td>Laplacian operator</td>
</tr>
<tr>
<td>(E)</td>
<td>Pa</td>
<td>Young’s modulus</td>
</tr>
<tr>
<td>(E)</td>
<td>(V/m)</td>
<td>analytic electric field magnitude</td>
</tr>
<tr>
<td>(E_C)</td>
<td>(V/m)</td>
<td>electric field magnitude at sharp corners</td>
</tr>
<tr>
<td>(E_{</td>
<td></td>
<td>})</td>
</tr>
<tr>
<td>(E_Y)</td>
<td>(V/m)</td>
<td>total electric field</td>
</tr>
<tr>
<td>(E)</td>
<td>(V/m)</td>
<td>electric field</td>
</tr>
<tr>
<td>(E_F)</td>
<td>eV</td>
<td>Fermi energy</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>–</td>
<td>strain</td>
</tr>
<tr>
<td>(\epsilon_f)</td>
<td>–</td>
<td>strain at failure</td>
</tr>
<tr>
<td>(\epsilon_{uts})</td>
<td>–</td>
<td>ultimate tensile strain</td>
</tr>
<tr>
<td>(\epsilon_{ys})</td>
<td>–</td>
<td>strain at yield</td>
</tr>
<tr>
<td>(\epsilon_i)</td>
<td>(C/Vm)</td>
<td>electric permittivity of material (i)</td>
</tr>
<tr>
<td>(\epsilon_o)</td>
<td>(C/Vm)</td>
<td>electric permittivity of free space</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>–</td>
<td>strain matrix</td>
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### Table A.2: List of symbols and abbreviations (F-K)

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<td>( F )</td>
<td>N</td>
<td>applied force</td>
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<tr>
<td>( F_{\text{elect}} )</td>
<td>N</td>
<td>electrostatic force</td>
</tr>
<tr>
<td>( F_{\text{iner}} )</td>
<td>N</td>
<td>inertial force</td>
</tr>
<tr>
<td>( F_K )</td>
<td>N</td>
<td>restoring/spring force</td>
</tr>
<tr>
<td>( F_{\text{VDW}} )</td>
<td>N</td>
<td>van der Waals force</td>
</tr>
<tr>
<td>( g )</td>
<td>m, um, nm</td>
<td>gap height</td>
</tr>
<tr>
<td>( g_0 )</td>
<td>m, um, nm</td>
<td>initial gap height</td>
</tr>
<tr>
<td>( G )</td>
<td>–</td>
<td>gate electrode</td>
</tr>
<tr>
<td>( G_W )</td>
<td>m, um, nm</td>
<td>gate width</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>–</td>
<td>tunneling parameter, number of atoms</td>
</tr>
<tr>
<td>( h )</td>
<td>Js</td>
<td>Planck’s constant</td>
</tr>
<tr>
<td>( \hbar )</td>
<td>Js</td>
<td>reduced Planck’s constant</td>
</tr>
<tr>
<td>( I )</td>
<td>( m^4 )</td>
<td>bending moment of inertia</td>
</tr>
<tr>
<td>( I )</td>
<td>A</td>
<td>current</td>
</tr>
<tr>
<td>( J )</td>
<td>–</td>
<td>Jacobian</td>
</tr>
<tr>
<td>( J )</td>
<td>( A/m^2 )</td>
<td>current density</td>
</tr>
<tr>
<td>( J_o )</td>
<td>( A/m^2 )</td>
<td>current density coefficient</td>
</tr>
<tr>
<td>( J )</td>
<td>( A/m^2 )</td>
<td>current density</td>
</tr>
<tr>
<td>( k_B )</td>
<td>J/K</td>
<td>Stefan-Boltzmann constant</td>
</tr>
<tr>
<td>( K_{\text{eff}} )</td>
<td>N/m</td>
<td>effective stiffness</td>
</tr>
<tr>
<td>( K_s )</td>
<td>N/m</td>
<td>spring stiffness</td>
</tr>
<tr>
<td>( K_\sigma )</td>
<td>N/m</td>
<td>stress contribution to stiffness</td>
</tr>
<tr>
<td>( K_T )</td>
<td>N/m</td>
<td>tangential stiffness matrix</td>
</tr>
<tr>
<td>( K_{\text{el}} )</td>
<td>N/m</td>
<td>elemental stiffness matrix</td>
</tr>
<tr>
<td>( K )</td>
<td>N/m</td>
<td>total stiffness matrix</td>
</tr>
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Table A.3: List of symbols and abbreviations (L-R)

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<tr>
<td>$l_{\text{detach}}$</td>
<td>m, um</td>
<td>detachment length</td>
</tr>
<tr>
<td>$L$</td>
<td>m, um</td>
<td>WALD structure length</td>
</tr>
<tr>
<td>$L$</td>
<td>$J$</td>
<td>Lagrangian</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>m</td>
<td>mean free path</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>–</td>
<td>eigen value</td>
</tr>
<tr>
<td>$m$</td>
<td>kg</td>
<td>mass</td>
</tr>
<tr>
<td>$m_e$</td>
<td>kg</td>
<td>electron mass</td>
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<tr>
<td>$M$</td>
<td>–</td>
<td>dimensionless mass</td>
</tr>
<tr>
<td>$M$</td>
<td>Nm</td>
<td>applied moment</td>
</tr>
<tr>
<td>$M_A$</td>
<td>Nm</td>
<td>reaction moment at pont A</td>
</tr>
<tr>
<td>$M_B$</td>
<td>Nm</td>
<td>reaction moment at pont B</td>
</tr>
<tr>
<td>$M_{\text{el}}$</td>
<td>kg</td>
<td>elemental mass matrix</td>
</tr>
<tr>
<td>$M$</td>
<td>kg</td>
<td>total mass matrix</td>
</tr>
<tr>
<td>$n$</td>
<td>–</td>
<td>index of refraction</td>
</tr>
<tr>
<td>$n$</td>
<td>$1/m^3$</td>
<td>carrier density</td>
</tr>
<tr>
<td>$n_{e}$</td>
<td>$1/m^3$</td>
<td>conducting electron density</td>
</tr>
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<td>$\nu$</td>
<td>–</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Hz</td>
<td>ionization frequency</td>
</tr>
<tr>
<td>$\mathbf{n}$</td>
<td>–</td>
<td>unit normal vector</td>
</tr>
<tr>
<td>$\mathbf{N}$</td>
<td>–</td>
<td>shape functions</td>
</tr>
<tr>
<td>$\phi$</td>
<td>eV</td>
<td>workfunction</td>
</tr>
<tr>
<td>$\psi$</td>
<td>m, um</td>
<td>discretize displacement</td>
</tr>
<tr>
<td>$\dot{\psi}$</td>
<td>m/s, um/s</td>
<td>discretized velocity</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>V</td>
<td>electric potential</td>
</tr>
<tr>
<td>$q$</td>
<td>C</td>
<td>charge</td>
</tr>
<tr>
<td>$q_e$</td>
<td>C</td>
<td>electron charge</td>
</tr>
<tr>
<td>$q_{el}^i$</td>
<td>C</td>
<td>$i$-th elemental parallel plate charge</td>
</tr>
<tr>
<td>$\Delta r_i$</td>
<td>m</td>
<td>average radial distance of nearest neighbors in direction $i$</td>
</tr>
<tr>
<td>$R$</td>
<td>–</td>
<td>resistance</td>
</tr>
<tr>
<td>$R$</td>
<td>–</td>
<td>residual</td>
</tr>
<tr>
<td>$R_A$</td>
<td>N</td>
<td>reaction force at point A</td>
</tr>
<tr>
<td>$R_B$</td>
<td>N</td>
<td>reaction force at point B</td>
</tr>
<tr>
<td>$\rho$</td>
<td>kg/m$^3$</td>
<td>density</td>
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Table A.4: List of symbols and abbreviations (S-V)

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<tr>
<td>$S$</td>
<td>–</td>
<td>source electrode</td>
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<tr>
<td>$\sigma$</td>
<td>Pa</td>
<td>stress</td>
</tr>
<tr>
<td>$\sigma_{uts}$</td>
<td>Pa</td>
<td>ultimate tensile stress</td>
</tr>
<tr>
<td>$\sigma_{ys}$</td>
<td>Pa</td>
<td>yield stress</td>
</tr>
<tr>
<td>$t$</td>
<td>m, nm</td>
<td>WALD thickness</td>
</tr>
<tr>
<td>$t$</td>
<td>s</td>
<td>time</td>
</tr>
<tr>
<td>$T$</td>
<td>s</td>
<td>characteristic time</td>
</tr>
<tr>
<td>$T$</td>
<td>K, C</td>
<td>temperature</td>
</tr>
<tr>
<td>$T$</td>
<td>–</td>
<td>transmission coefficient</td>
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<tr>
<td>$T$</td>
<td>J</td>
<td>total kinetic energy</td>
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<tr>
<td>$T_{el}$</td>
<td>J</td>
<td>elemental kinetic energy</td>
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<td>$\theta_i$</td>
<td>rad</td>
<td>rotation resulting from applied moment $M_i$</td>
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<td>$\Theta$</td>
<td>–</td>
<td>tunneling model correction factor</td>
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<tr>
<td>$\Theta_{NM}$</td>
<td>–</td>
<td>NL Newmark correction factor</td>
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<td>$\tau$</td>
<td>–</td>
<td>dimensionless time</td>
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<td>$u$</td>
<td>m, um</td>
<td>displacement</td>
</tr>
<tr>
<td>$u$</td>
<td>–</td>
<td>dimensionless displacement</td>
</tr>
<tr>
<td>$u_i$</td>
<td>m</td>
<td>displacement resulting from applied force $F_i$</td>
</tr>
<tr>
<td>$\bar{u}_i$</td>
<td>m</td>
<td>average center point displacement of element $i$</td>
</tr>
<tr>
<td>$U_{el}$</td>
<td>$J/m^3$</td>
<td>volumetric potential energy</td>
</tr>
<tr>
<td>$U$</td>
<td>J</td>
<td>total potential energy</td>
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<tr>
<td>$U_{el}$</td>
<td>J</td>
<td>elemental potential energy</td>
</tr>
<tr>
<td>$v$</td>
<td>m/s</td>
<td>velocity</td>
</tr>
<tr>
<td>$v_e$</td>
<td>m/s</td>
<td>Fermi velocity</td>
</tr>
<tr>
<td>$V$</td>
<td>V</td>
<td>applied voltage</td>
</tr>
<tr>
<td>$V_{DD}$</td>
<td>V</td>
<td>maximum supply voltage</td>
</tr>
<tr>
<td>$V_{DS}$</td>
<td>V</td>
<td>potential applied between drain and source</td>
</tr>
<tr>
<td>$V_{GS}$</td>
<td>V</td>
<td>potential applied between gate and source</td>
</tr>
<tr>
<td>$V_{pullin}$</td>
<td>V</td>
<td>pull-in/actuation voltage</td>
</tr>
<tr>
<td>$V_{SS}$</td>
<td>V</td>
<td>minimum supply voltage</td>
</tr>
<tr>
<td>$V_o$</td>
<td>eV</td>
<td>potential barrier height</td>
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Table A.5: List of symbols and abbreviations (W-Y)

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<th>Symbol</th>
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<tr>
<td>w</td>
<td>m, um, nm</td>
<td>width</td>
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<tr>
<td>$W_o$</td>
<td>m, um</td>
<td>bow/poly-tie minimum half-width</td>
</tr>
<tr>
<td>$W_M$</td>
<td>m, um</td>
<td>bow/poly-tie maximum half-width</td>
</tr>
<tr>
<td>$\xi$</td>
<td>N/m</td>
<td>distributed load</td>
</tr>
<tr>
<td>y</td>
<td>m</td>
<td>displacement</td>
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Appendix B

Irradiated CMOS

B.1 CMOS Scaling

Robert Dennar of IBM’s T.J. Watson Research Center was the first researcher to propose an effective scaling algorithm for MOS transistors that was capable of improving both performance and density [24]. The algorithm is as follows: reduce the transistor dimensions (channel length, channel width, gate oxide thickness) and power supply by some factor $S$, where $S < 1$. A diagram for an NMOS transistor in the off-state and a CMOS transistor set are shown in figures B.1 and B.2. In doing so it can be shown that the device footprint is reduced by a factor of $S^2$, the switching speed improved by the factor $S$, and the actuation energy reduced by a factor of $S^3$.

Following Dennars scaling law, devices were successfully scaled by a factor $S = 0.7$ per generation until the 130 nm design node at which point the aforementioned physical scaling limit was reached. Forty years ago the transistor’s minimum layout dimensions were 10 µm, and today they are 35 nm with the 45 nm generation of processors [25, 164]. Scaling of the lateral dimensions of the channels and gates has continued in parallel with the advancements in batch lithography processes. In 1998 the lithography energy source for the 250 nm technologies was deep ultra-violet (DUV) laser light with a wavelength of 248 nm, and today the state-of-the-art lithography techniques implement advanced immersion technologies [164].

For the past 40 years the insulator of choice for MOS technologies has been $SiO_2$. The
oxide has been used as the field oxide, which separates the individual transistors, and as the gate oxide. With continued scaling the thickness of the gate oxide decreased from 100 nm to only a handful of atoms. In 2003 at the 90 nm generation the thickness of the $SiO_2$ hit 5 atoms in thickness, as such there was no scaling of the oxide thickness from the 90 nm to
the 65 nm nodes [25]. Scaling issues involving the gate oxide include dielectric break down because the electric-field increases with decreasing gate thickness, and electron tunneling which begins occurring when gate oxide thicknesses are < 2 nm. Thus, at thickness of only 5 atoms the $SiO_2$ essentially ran out of atoms, the material ceased to serve as an insulator between the gate and the conducting channel, and electrons were able to tunnel from the gate to the conducting channel. The resulting increase in power consumption resulted in the production of laptops that drained their batteries too quickly, and microprocessors whose cooling demands became increasingly difficult to meet.

After the 90 nm technology node Intel began to investigate solutions to the gate-oxide scaling problem. As of the 45 nm node, which began production in January 2007, Intel began using high k + metal gate/gate-oxide pairings in their CMOS transistors [25, 99]. K, the dielectric constant, is related to the polarizability of the material [80]. When a dielectric is placed in an electric field, such as the one that results from the charges stored between the parallel plates, its molecules align with the electric field. The larger the dielectric constant of the dielectric material, the more responsive is the material to the electric field. Thus, when a material has a high k value it means that it can provide increased capacitance between conducting plates, allowing for more charge to be stored. Therefore by choosing a new insulating material with a higher k, the gate-oxide thickness can be increased, leakage currents reduced, power dissipation reduced, device performance increased, and future scaling practices maintained.

While solving the oxide scaling problem Intel investigated an array of high k dielectrics including: $Al_2O_3$, $TiO_2$, $Ta_2O_5$, $HfO_2$, $HfSiO_4$, $ZrO_2$, $ZrSiO_4$, $La_2O_3$ [25]. Furthermore, it was found that prototype transistors fabricated by replacing the $SiO_2$ gate oxide with Hf and Zr based oxides performed worse than their traditional MOSFET counterparts. The transistors suffered from Fermi-pinning, charge-trapping, and lower carrier mobility, resulting from phonon scattering. Because it was found that charge-trapping density was dependent on surface roughness, charge-trapping problems were solved by choosing to use atomic layer
deposited materials which are known to be perfectly conformal, extremely smooth, i.e. have a low RMS surface roughness value, and pin hole free [121, 83, 229, 193, 227]. Computer models of the devices revealed that the problems related to Fermi-pinning and phonon scattering could be solved by replacing the poly-silicon gates with metal gates whose work functions closely match those of the N/PMOS conducting channels [25]. In the end, 1.0 nm thick Hf based high k gate dielectrics deposited via ALD were chosen to replace $SiO_2$ in the 45 nm design node. The high-k + metal gate provided a dramatic decrease in gate leakage. Gate leakage was reduced by $>25X$ for NMOS and by 1000X for PMOS transistors [164].

Continued scaling of CMOS technology requires lower supply voltages, decreased threshold voltages, ever thinning gate oxides, and decreased device dimensions, resulting in increasingly insurmountable fabrication problems. While it appears that a perfectly adequate materials based solution has been found, and the 40 year march of Moores law can proceed uninterrupted, the solutions are merely temporary and allow for only a couple more technology nodes before designers encounter yet again gate-oxides that are too thin, and are thus forced to search for increasingly exotic high k + metal combinations.

B.2 Irradiation of MOS Devices

The transient material/device response of MOS transistors to ionizing radiation is very complex, depending on applied bias, temperature, dose rate, and annealing time. The entire response time scale of an irradiated device may span many decades of time – from $10^{-12}$ to $10^6$ seconds [176, 172, 175, 214, 160]. The basic radiation damage to MOS devices is the buildup of electrically active defects at or near the oxide/Si interface, figure B.3. Total irradiation dose effects include the modification of device structure and the introduction of charge accumulation (traps) in critical regions of the device – specifically, the field oxide and gate oxide. The effect of ionizing radiation on the gate oxide in a CMOS device is radiation-induced charge trapping. The trapped charges build up in the gate oxide and cause a shift in the threshold voltage [208, 87, 161], which is the voltage that must be applied to turn the
device on. If the shift is great enough the device cannot be turned off, and the device is said to have experience failure via depletion mode [176].

![Figure B.3: Schematic of n-channel MOSFET illustrating radiation-induced charging of the gate oxide: a) normal operation and b) post-irradiation [176]](image)

The magnitude and permanency of the sub-threshold shift depends on several factors including: gate oxide thickness, field strength, and level of radiation exposure. Some of the radiation induced defects in the gate oxide, including trapped positive charges (holes) can be annealed, resulting in recovery of the threshold voltage known as rebound, or in some cases super-rebound, in which the post-radiation threshold voltage recovers to a value greater than that of the un-irradiated device [172, 175, 176, 191]. The annealing process can be thermally activated, called thermal de-trapping, or at lower temperatures accomplished via electron tunneling [19, 35, 175, 176, 191, 214].

As scaling efforts have continued to follow the beat of Moore’s drum, gate oxides have become ultra-thin, resulting in negligible sub-threshold voltage shifts thanks in part to the increased efficiency of annealing via tunneling. Essentially, super-thin layers are incapable of trapping high concentrations of holes, because the oxide thickness is of the same order as the tunneling front [191, 214], therefore the trapped holes in the gate oxide are easily annihilated (neutralized) by electrons tunneling from the Si substrate. Thus, todays CMOS technologies have gate oxides considered to be inherently radiation hard [159, 175, 176]. However, as
the gate oxide thickness decreases and MOS devices become increasingly radiation-hard, the primary source of device failure comes from radiation damage to the separation (field) oxide, which has necessarily remained much thicker than the gate oxide. Just as seen in gate oxides, in the field oxide ionizing radiation is responsible for the generation of point defects, such as single atom displacements, or electron-hole pairs, and also large regions of disorder that contain high densities of defects, which are more prone to charge trapping. Because charge generation per dose of radiation is dependent on the thickness of the irradiated oxide the voltage shift seen in the field oxide is much greater, and thus the leakage current directly affects the device characteristics. Charge buildup in the field oxide results in parasitic leakage paths for electrons from the source-to-drain outside of the active gate region, figure B.4. The effects of the charge build-up in the field oxide on the IV characteristics of an NMOS transistor are show in B.5.

Figure B.4: Schematic illustration of the LOCOS field oxide isolation structure and possible leakage paths [175]

Recently (2009), Xue et al. studied irraditated CMOS transistors with ultra-thin SiO₂ gate oxides (∼ 3.5 nm) and found that the holes trapped by the irradiated field oxide, figure
B.6, cause shifts in saturation current, figure B.7, shifts in transconductance, figure B.8, and an increase in off-state current [232]. After irradiation the NMOS transconductance peak drops in magnitude by 14.8%, the off-state current is seen to increase a full order of magnitude, and a slight increase in the sub-threshold swing is observed. The increase in off-state current is attributed to a build up of positive charge in the shallow trench isolation. The $I_{ds}-V_{ds}$ plots show a decrease in $I_{ds}$ for all $V_{ds}$, figure B.7. There is no evident change in threshold voltage, indicated by a shift in $g_m$ vs. $V_{ds}$, figure B.8.

After irradiation the PMOS transconductance peak drops by 30.7% and shifts to a negative value of $V_{gs}$. The change in magnitude of the transconductance peak is greater than that for NMOS transistors. The threshold voltage was seen to shift negatively by 160 mV. Furthermore, a large decline in saturation drain current was observed, up to 40%, figure B.7.

To some extent, the same annealing mechanisms active in the gate-oxide are also active in the field oxide – with the exception of ambient-temperature thermal de-trapping. In 1989 Terrell et al [214] saw that that thermal de-trapping was observed only at elevated
Figure B.6: Positive charges trapped in the spacers and its effects for NMOSFETs and PMOSFETs [232]

Figure B.7: a) $I_{ds} - V_{ds}$ characteristics before and after proton exposure $1 \times 10^{15}$ protons/cm$^2$ for NMOSFETs with W/L=0.22/0.18 µm; b) $I_{ds} - V_{ds}$ characteristics before and after proton exposure $1 \times 10^{15}$ protons/cm$^2$ for PMOSFETs with W/L=0.22/0.18 µm. [232]
temperatures, whereas thermal de-trapping is seen in gate oxides at room temperature. This was attributed to the difference in thickness between the two oxides. The density of trapped charges per dose of radiation is greater for thick layers of oxide. Therefore, when comparing super thin gate oxides and thicker field oxides, proportionally fewer holes are removed at room temperature, and thus thermal annealing at room temperature has only a negligible effect on recovery. Thus, depending on operating conditions (radiation dosage, temperature, field strength), the type of damage reported by Xue et al may be recoverable to some extent.
However, as device parameters such as the threshold voltage, and power budget become less malleable and insensitive to variation, small shifts in parameters such as saturation voltage, off-state current, and transconductance may still cause failure.

B.2.1 Radiation Induced Leakage Current and Carrier Mobility Degradation

As device dimensions continue to scale, two additional radiation effects capable of causing CMOS device failure need be considered, namely, radiation induced leakage current (RILC) and carrier mobility degradation. The main reliability concern in irradiated MOS devices with ultra-thin gate oxides is low-field gate leakage current, as measured after exposure to radiation or electrical stress, i.e., radiation induced leakage current (RILC), or stress induced leakage current (SILC) [35]. RILC can best be described as an inelastic tunneling process, meaning the electron loses energy, $\approx 1$ eV, mediated by neutral traps in the gate oxide [192]. When positive traps are created in the gate oxide, electrons from the substrate can tunnel to these trap states, and then tunnel from the trapped states to the gate. In other words, one can think of RILC as controlled by the flux of holes, generated by impact ionization or ionizing radiation, across the gate oxide.

The applied gate bias during irradiation has been observed to heavily influence the magnitude of RILC. In 1997 Scarpa et al. [192] showed for the first time that radiation (gamma from a $^{60}$Co source) can induce leakage current in very thin oxides ($t_{ox} < 4.5$ nm), finding that RILC was greatest for positive/negative applied biases whose magnitudes were close to 0 Volts, and that the magnitude of RILC decreased with increasing magnitude of applied bias, with the increase in RILC most dramatic for a negative bias, figure B.9. In 1998 Cescia et al. confirmed the findings of Scarpa using an 8 MeV electron radiation source, finding RILC to be field dependent in ultra-thin oxides ($\sim 4$ nm) [35]. They observed that RILC was a maximum for a device with zero bias during irradiation, while RILC for devices irradiated under a positive, or negative bias, decreases for an increasing electric-field. This phenomenon has been attributed to the creation of holes that drift near either an anode or
cathode interface due to the applied field, which in turn creates a larger localized density of traps, which are neutralized via recombination or tunneling.

![Graph](image)

Figure B.9: Gate currents in the RILC regime after a 5.3 Mrad(Si) gamma dose; (a) positive currents; (b) negative currents, for different bias conditions during irradiation, as listed: [192]

Finally, radiation induced defects near the gate oxide/Si interface can act as scattering centers to reduce carrier mobility in the conducting channel, thereby reducing operational current levels in the device [175, 176]. In 1980 Sun et al. gave a comprehensive review of different scattering mechanisms, observing that for MOSFETS at room temperature and near the threshold voltage, carrier mobility is mainly governed by coulombic and phonon scattering [206]. Essentially, the build-up of trapped holes near the gate oxide/Si interface creates more scattering centers that hamper the mobility of the carriers in the conducting channel, thereby causing a notable decrease in the transconductance of the device, as seen in the work by Xue et al. [160].
B.3 Micro to Nano Via Fabrication

B.3.1 Top-down and Pertinent Nano-capable Lithography Techniques

Nano-technology is a broad and rapidly developing field of science. Nano-technology’s origins are rooted in many different sciences and disciplines, including: physics, chemistry, biology, material science, mechanical engineering, electrical engineering and aerospace engineering, to name a few [150, 21, 141, 124, 225, 74, 153, 145, 32, 235, 234, 16, 221, 50]. The field of NEMS was born from years of development in the microelectronics and MEMS industries [49]. At the most basic level one can think of NEMS as the miniaturization of already minute MEMS devices. Whereas MEMS devices tend to be on the micro scale ($10^{-6} - 10^{-2}$ m) [90], NEMS devices contain features less than 100 nm in size. It follows that the fabrication techniques to produce such fine features are both technically challenging and limited. Not all fabrication techniques developed to date in the MEMS and semiconductor industries are capable of fabricating nano-structures [49]. For example, traditional optical lithography techniques commonly used in both industries cannot produce features on the nano scale because the optical lithography process is limited by the wavelength of the light used to expose photoresist [222, 220]. The wavelength of near ultra-violet (NUV) light, the typical light source for optical lithography, is approximately 400 - 200 nm, thus nano scale features cannot be achieved without modifications to the process. Techniques that have demonstrated the capability to create nano scale features have been grouped into three categories: direct, indirect and self-assembly [49].

Direct nano-fabrication techniques include modified optical lithography processes such as immersion lithography [23] and extreme ultra-violet lithography (EUV) [139, 199, 79, 14], as well as a set of processes known as next generation lithography (NGL). Next generation lithography encompasses processes such as electron beam lithography (EBL) [220, 158, 46] and focused ion-beam lithography (FIB) [155, 156, 10]. As previously mentioned, conventional lithography techniques are theoretically limited by a one-to-one relationship between
feature size and electro-magnetic wavelength. Modern lithography techniques like immersion lithography are capable of producing features as small as 32 nm [49]. This process replaces a gap of air between the focusing lens and substrate with a liquid having an index of refraction greater than 1. By employing this method the feature resolution is reduced by a factor equal to the refractive index of the medium [23]. Other direct lithography techniques such EUV (wavelengths of approximately 1-30 nm) operate based on essentially the same principle as traditional optical lithography, but because EUV wavelengths are much smaller than the those of UV light it is possible to create nano scale features.

Direct writing is the most common EBL approach. It has been used for a variety of applications since the late 1960’s. EBL is a very high resolution process that, when combined with etching and deposition processes, allows fabrication of devices with critical dimensions as small as 10 nm [220]. In EBL a focused beam of electrons is used to expose a photoresist in the same way that light is used to expose film or UV sensitive photoresist in optical lithography. The resolution of EBL is limited by electron scattering in the photoresist. This occurs because the high-energy electrons tend to bounce around inside of the photoresist in close proximity to the desired pattern area. When this occurs the photo resist is damaged wherever the electrons have traveled, thereby diminishing the definition of the intended pattern. When electron scattering is severe it produces what appears to be a halo around the developed pattern. This halo effect can be minimized by adjusting other parameters of the EBL machine including electron energy, beam spot size, and dosage.

Similar to EBL, focused ion beam lithography uses a beam of focused ions to create patterns. FIB has advantages over EBL in that it combines lithography and pattern transfer in one tool. Structures can be created on a substrate by sputter etching or ion/electron induced deposition [49]. FIB does not have as high a resolution as EBL, only 30 nm compared to 10 nm, but because it is more versatile in its processing capabilities FIB has proven to be a superior choice for direct nano-fabrication. Because NGL processes are limited by throughput capability, applications have mainly been limited to mask production,
prototyping, fabrication of small volume special products, and research and development for advanced applications.

Some other methods of direct nano-fabrication lithography that have not been mentioned here include nano-imprinting (soft-contact techniques) [242] and scanning probe lithography [222]. The fundamental feature size limits for these methods, as well as the processes discussed, are shown in figure B.10.

![Fabrication technique and their dimensional limits](https://via.placeholder.com/150)

Figure B.10: Fabrication technique and their dimensional limits [49]

Indirect nano fabrication techniques take advantage of lateral etching. The etching can be either a dry etch, typically reactive ion (RIE), or a wet etch (chemical etching). With these methods a pattern is developed using a suitable lithography technique and then the desired device geometry is created via lateral etching, which results in an undercut of the original pattern. This method is the same used to fabricate micro-needle arrays, where the tip of the micro needle may have a diameter smaller than 100 nm, classifying it as a nano-scale feature.

### B.3.2 Bottom-up

Self-assembly refers to devices created by the self-assembly of molecules. Nano-fabrication by molecular self-assembly is also called ”bottom-up” fabrication, and the direct methods known as ”top-down” fabrication [49]. The most common bottom-up nano-fabrication pro-
cess used in NEMS devices is the growth of carbon nano tubes (CNTs). Several NEMS devices have been demonstrated using CNTs, including vertically aligned capacitive CNT nano-switches and resonators [135, 61, 117, 55]. The disadvantage of self-assembly methods is that molecules tend to grow in random orientations [103, 49]. In practice it is extremely difficult to grow a sing nano-tube in a specific orientation. To overcome this obstacle CNTs are typically grown in bundles. Because of the current difficulty in creating NEMS devices based on a self-assembly method, NEMS sensors, and switches based on this method, do not yet have commercially viable applications.

**B.3.3 Thin-film Sacrificial Layers**

Sacrificial layers are widely used in micro and nano surface micro-machining processes for the fabrication of MEMS and NEMS devices capable of both in and out of plane motion. The purpose of a sacrificial layer is to create gaps between features. These gaps serve varying purposes depending on the device, including allowing for mechanical functionality, separating charge between surfaces, and creating thermal isolation. A great variety of materials are used as sacrificial layers, ranging from a broad selection of metals to ceramics and polymers. There are several commonly employed methods for deposition of sacrificial layers: physical vapor deposition (PVD), chemical vapor deposition (CVD), and spin casting [196], each of which have made the leap from micro to nano-fabrication processes [202, 42, 117, 54, 52].

PVD evaporation, thermal or electron beam, allow for controlled thin-film deposition of most metals. Depending on chamber size and material, thermal evaporation may be low temperature or high temperature. As an alternative electron-beam evaporation is preferable when a low temperature deposition is required, or a refractory material is to be evaporated [70]. Tanner and Rogers have successfully fabricated cantilever devices with integrated tunnel junctions employing a 60 nm sacrificial layer of Al deposited by electron-beam evaporation on top of 250 nm electrodes [212].

CVD thin film deposition techniques are common in widely used commercial processes
such as SUMMiT and MUMPS [44], and offer a more conformal coating than PVD techniques. CVD produces near conformal films that tend to yield rounded corners and dimples when deposited on top of existing features [166]. Both metals and different ceramics can be deposited using CVD techniques. Common ceramics include poly-silicon, silicon dioxide, and nitride, and CVD deposit-able metals include Ni, Mo, Ta, and W. Recently Kim et al. produced a 10 nm thick, continuous, dense and conformal layer of Cu having an RMS roughness of $\sim 1$ nm [118]. Choi and King were able to create spacers for nanoscale CMOS technology using 10-30 nm thick LPCVD deposited PSG sacrificial layers, but reported only 70% step coverage over a feature having a thickness of 20-30 nm [42]. Kaul et al. demonstrated that a 200 nm thick layer of silicon dioxide deposited by PECVD could be thinned down to 20 nm and used as a sacrificial layer for electromechanical carbon nanotubes switches [117].

Other methods for using polymers such as PMMA and PMGI sacrificial layers have been successfully demonstrated [135, 237]. Young et al. demonstrated MEMS resonators using 100-240 nm thick spin-coated PMGI as a sacrificial layer [237]. These devices however suffered from poor step coverage, and with a sacrificial layer of 120 nm reported only a 22% yield of functioning devices. Lee et al. have demonstrated suspended carbon nano relays using a 150 nm thick layer of spin-coated PMMA deposited on top of 15 nm thick actuation electrodes for a sacrificial layer [135].

The methods introduced for deposition of sacrificial layers for use in the development of MEMS or NEMS devices all face serious limitations as the layers approach nanoscale thickness. The downside of PVD evaporation is its poor step coverage of existing features. Because of geometrical shadowing caused by existing structures, the resulting thin film will be preferentially deposited on the top and top corners of the existing features. Consequently, the step coverage is particularly poor at the bottom corner of trenches and vias [116]. Thus the ratio of film feature thickness to gap width of existing features limits the application of PVD deposited sacrificial layers. It has been shown that oblique angle physical evaporation can significantly improve the step coverage limitations of PVD evaporation [116]. It should
be noted that PVD sputtering typically allows for better step coverage than evaporation and a larger selection of materials such as ceramics [147]. CVD has several limitations; the method offers better step coverage than PVD techniques, but the process cannot produce ideally conformal thin films. In addition, many CVD processes are high temperature. This limits use of patterning materials such as resists, and induces thin film stress, which may be deleterious to device performance. Polymers, as sacrificial materials, offer simple and low temperature process. However, these materials, because of spin or dry-coating processes, suffer from poor step coverage, and the nature of the deposition makes exact control of the film thickness impossible. Fortunately, atomic layer deposition (ALD) is an emerging thin film direct-growth process that can circumvent the aforementioned limitations when implemented at low temperatures. In fact ALD $Al_2O_3$ has been used to produce sacrificial layers of only 10 nm between 250 nm thick poly-silicon and 15 nm thick gold electrodes, demonstrating the awesome step coverage capabilities of ALD thin films [178].
Appendix C

Approximation of Hamaker Constants via Lifshitz Theory

C.1 Van der Waals Interaction and Hamaker Approximations via Lifshitz Theory

Van der Waals energy/force arises from the interaction of two materials across a third medium which is either a liquid, gas, or vacuum. The van der Walls interaction results from electrodynamic interactions between oscillating and/or rotating electrical dipoles within the interacting media [162]. This interaction produces attractive or repulsive forces between interacting media. In the case of attractive forces, which are most common, if the magnitude of the force is large enough stiction may occur.

There are two methods used to calculate the interaction energies/forces between material systems. The first method considers dipole interactions of molecular pairs at a microscopic level. This approach can become quite complex when considering the interaction of neighboring molecules on the interaction of interacting pairs. The second approach, developed by Lifshitz, allows the van der Waals interaction energy and forces to be calculated via macroscopic material properties and geometry. Lifshitz theory neglects the atomic structure of materials completely, instead solids are treated as continuous materials with bulk properties, for example the dielectric permittivity and the refractive index [31]. A more detailed description of both of these theories and their applications can be found in [31].

The van der Waals force is directly proportional to a material-system dependent constant called the Hamaker constant, and inversely proportional to the separation distance
for two interacting surfaces, equation C.1. Therefore interaction forces become increasingly large as separation distances decrease. Now, typical MEMS and NEMS systems have separation distances between structures ranging from a few microns to a few nanometers. If these separation distances are between deformable structures, as is the case for electrostatically actuated switches, significant static deflection of the deformable structure may occur. Furthermore, depending on device specific parameters, such as the interacting material system, which effects the magnitude of the Hamaker constant, the separation distance between structures, and the stiffness of the structures, the devices may experience un-biased pull-in, and thus failure. It is for this reason that the van der Waals force and its effect on micro and nano scale systems, should be regarded as a design parameter for MEMS and NEMS systems.

\[ F_{vdw} = \int \frac{A_{132}}{6\pi y^3} dA \] (C.1)

In the following Lifshitz theory will be used to derive analytic equations for calculating the Hamaker constant for three different material systems particularly relevant to MEMS and NEMS. The material systems considered are: metal₁ − vacuum/air − metal₂, metal₁ − vacuum/air − metal₁, and ceramic − vacuum/air − metal₂. From these equations the Hamaker constant, and thus van der Waals force for any number of MEMS/NEMS devices, may be approximated.

The expression for the Hamaker constant developed by Lifshitz is given in equation C.2, [31]. From equation C.2 we see that the Hamaker constant is dependent on the static and frequency dependent permittivity of the interacting media.

\[ A_{132} = \frac{3}{4} k_b T \left( \frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right) \left( \frac{\epsilon_2 - \epsilon_3}{\epsilon_2 + \epsilon_3} \right) + \frac{3h}{4\pi} \int_{\nu_o}^{\infty} \left( \frac{\epsilon_1 (i\nu) - \epsilon_3 (i\nu)}{\epsilon_1 (i\nu) + \epsilon_3 (i\nu)} \right) \left( \frac{\epsilon_2 (i\nu) - \epsilon_3 (i\nu)}{\epsilon_2 (i\nu) + i\epsilon_3 (i\nu)} \right) d\nu \] (C.2)

where, \( \nu_1 = \frac{2\pi k_b T}{h} \approx 3.9 \cdot 10^{13} \text{ Hz at } 25^\circ \text{ C.} \)
\[
\epsilon(i\nu) = 1 + \frac{n^2 - 1}{1 + \nu_e^2}
\]  \hspace{1cm} (C.3)

\[
\epsilon(i\nu) = 1 + \frac{\nu_e^2}{\nu^2}
\]  \hspace{1cm} (C.4)

In equation C.3 \(n\) is the refractive index and \(\nu_e\) the mean ionization frequency of the dielectric material, and in equation C.4 \(\nu_e\) is the plasma frequency of the electron gas [31] of the metal. We approximate the plasma frequency of the gas as the ionization frequency of the metal. Thus \(\nu_e\) can be calculated from C.5, where \(\phi\) is the work function of the metal.

\[
\phi = h\nu
\]  \hspace{1cm} (C.5)

C.2 Analytic Derivations for Different Material Systems Applicable to Thin-film NEMS devices

Using equations C.2-C.4 we can derive analytic expressions for several material systems relevant to thin-film NEMS devices. In the following subsections analytic expressions for the Hamaker constant of various material systems are derived. Material systems considered are as follows: \(metal_1 – vacuum/air – metal_2, metal – vacuum – metal, and metal – vacuum/air – dielectric\).

C.2.1 Metal-Vacuum/Air-Metal

For air or vacuum \(\epsilon_3 = \epsilon_3(i\nu) \approx 1\), and because the materials interacting across medium 3 are metals, we will use equation C.4 to approximate the dynamic dielectric constants. First, we will consider the case of dissimilar metals interacting across a medium of either vacuum or air: \(\epsilon_1 \neq \epsilon_2\) and \(\nu_1 \neq \nu_2\).

Using equation C.4 with equation C.2 we arrive at the following form of equation C.2 for the Hamaker constant,
\[ A_{132} = \frac{3}{4} k_b T \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right) \left( \frac{\epsilon_2 - 1}{\epsilon_2 + 1} \right) + \frac{3h}{4\pi} \int_{\nu_o}^{\infty} \frac{\nu_1^2 \nu_2^2}{\left( 2 + \frac{\nu_1^2}{\nu_2^2} \right) \left( 2 + \frac{\nu_2^2}{\nu_1^2} \right)} d\nu \]

Now, for a conductor the static dielectric constant \( \epsilon \to \infty \), therefore evaluating the above equation and taking the limit of the static term as the dielectric constants approach infinity we arrive at equation C.6, the analytic equation for calculating the Hamaker constant for two different metals interacting across a medium of either air or vacuum.

\[ A_{132} = \frac{3}{4} k_b T \lim_{\epsilon_1, \epsilon_2 \to +\infty} \left( \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right) \left( \frac{\epsilon_2 - 1}{\epsilon_2 + 1} \right) + \frac{3h}{4\pi} \lim_{A \to \infty} \left[ \frac{\nu_1 \nu_2 \left( \nu_1 \arctan \left( \frac{\sqrt{2} \nu}{\nu_1} \right) - \nu_2 \arctan \left( \frac{\sqrt{2} \nu}{\nu_2} \right) \right) - \sqrt{2} (\nu_1^2 - \nu_2^2) \right] \right] \]

Next, we consider the case for two like metals interacting across either vacuum or air: \( \nu_1 = \nu^2 \) and \( \nu_1 = \nu_2 \). As before, using equation C.4 with equation C.2 we find:

\[ A_{131} = \frac{3}{4} k_b T \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right)^2 + \frac{3h}{4\pi} \int_{\nu_o}^{\infty} \frac{\nu_1^2}{\nu_1^2 + 2\nu^2} d\nu \]

\[ A_{131} = \lim_{\epsilon_1 \to +\infty} \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right)^2 + \lim_{A \to +\infty} \left[ \frac{1}{4} \nu_1 \left( \frac{2\nu_1 \nu + \sqrt{2} (\nu_1^2 + 2\nu^2) \arctan \left( \frac{\sqrt{2} \nu}{\nu_1} \right) \right) \right] \]

\[ A_{131} = \frac{3}{4} k_b T + \frac{3h}{4\pi} \left[ \frac{1}{4\sqrt{2}} \frac{\nu_1^2 \nu_2^2}{\nu_1^2 + \nu_2^2} - \frac{\nu_1 \left( 2\nu_1 \nu_o + \sqrt{2} (\nu_1^2 + 2\nu^2) \arctan \left( \frac{\sqrt{2} \nu_o}{\nu_1} \right) \right)}{4 (\nu_1^2 + 2\nu^2)} \right] \quad \text{(C.7)} \]

C.2.2 Metal-Vacuum/Air-Ceramic

For a dielectric interacting with a metal across either vacuum or air we will use both equation C.3 and C.4 with equation Lifshitz to derive the analytic expression for the Hamaker constant. Thus, for this system we have,
\[ \epsilon_1(i\nu) = 1 + \frac{n^2 - 1}{1 + \frac{\nu^2}{\nu_c^2}} \]

\[ \epsilon_2(i\nu) = 1 + \frac{\nu_c^2}{\nu^2} \]

and again, \( \epsilon_3 = \epsilon(i\nu)_3 \approx 1. \)

Now, using these approximations for the frequency dependent permittivities, equation C.2 takes the form,

\[ A_{132} = \frac{3}{4} k_b T \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right) \left( \frac{\epsilon_2 - 1}{\epsilon_2 + 1} \right) + \frac{3h}{4\pi} \int_{\nu_0}^{\infty} \frac{\nu_2^2 (n^2 - 1)}{\nu^2 \left( 1 + \frac{\nu_2^2}{\nu_1^2} \right) \left( 2 + \frac{n^2 - 1}{\nu_1^2} \right)} d\nu \quad (C.8) \]

\[ \Rightarrow A_{132} = \frac{3}{4} k_b T \lim_{\nu_2 \to \infty} \left[ \left( \frac{\epsilon_1 - 1}{\epsilon_1 + 1} \right) \left( \frac{\epsilon_2 - 1}{\epsilon_2 + 1} \right) \right] + \frac{3h}{4\pi} \lim_{\nu_2 \to \infty} \left[ \frac{\nu_2 \arctan \left( \frac{\sqrt{2}\nu}{\nu_1 \sqrt{1 + n^2}} \right)}{\sqrt{2}(n^2 - 1) - \nu_2^2} \right] \left( \frac{\nu_1 \arctan \left( \frac{\sqrt{2}\nu}{\nu_1 \sqrt{1 + n^2}} \right)}{\sqrt{2}(n^2 - 1) - \nu_2^2} \right) \right] \]

\[ \Rightarrow A_{132} = \frac{3}{4} k_b T \frac{n^2 - 1}{\epsilon_1 + 1} + \frac{3h \nu_1 \nu_2 (n^2 - 1)}{4\sqrt{2}\pi (\nu_1^2 (1 + n^2) - \nu_2^2)} \left[ \nu_1 \nu_2 \frac{\sqrt{\nu_1 \nu_2 (1 + n^2) - \nu_2^2}}{2} - \nu_1 \sqrt{1 + n^2} \arctan \left( \frac{\sqrt{2}\nu}{\nu_1 \sqrt{1 + n^2}} \right) - \nu_2 \arctan \frac{\sqrt{2}\nu}{\nu_2 \sqrt{1 + n^2}} \right] \]

\[ C.2.3 \quad \text{Approximating } A_{132} \text{ from Characterized } Ax3x \text{ Systems} \]

In the case that the Hamaker constants for two different material systems \( \{131\} \) and \( \{232\} \) have been experimentally characterized, the Hamaker constant of the composed system \( A_{132} \) may be approximated by equation C.9, [31].

\[ A_{132} \approx \sqrt{A_{131} A_{232}} \quad (C.9) \]

By using this approximation with Lifshitz theory it is therefore possible to reasonably approximate the interaction forces acting on uncharacterized MEMS and NEMS devices. For
example, the material system for the devices developed by this work is WALD-vacuum/air-Au. The van der Waals interaction of this specific material system has not yet been reported, however Au-vacuum/air-Au systems are well characterized, with $A_{232} \approx 50 \cdot 10^{-20}$ J. Therefore the Hamaker constant for the unknown WALD-vacuum/air-Au system can be approximated by using equation C.9 with $A_{131}$ calculated using equation C.7, and $A_{232}$ the experimentally characterized Hamaker constant of Au-vacuum/air-Au system. The Hamaker constant for the WALD-vacuum/air-Au material system has thus been calculated to be $\approx 22 \times 10^{-20}$ J, which corresponds well with experimentally characterized metal-metal systems.
Appendix D

Cavitation/RIE Characterization

D.1 A 2nd Characterization of Cavitation/RIE Effects

Prior to fabrication a second characterization study of effects of cavitation/RIE on fabricated electrode geometries was conducted. The study was necessary because the glass plate that was in the RIE system during the first 3 years of the research effort was broken in early 2010. As a result the system became noticeably unstable and all previously characterized etch-rates became un-reliable. This was first discovered after fabrication of the WALD NEMS bow-tie devices, as is evident by their overlapping electrodes 5.27. Because I did not have a large number of chips available to me to characterize the process as before, section 5.7, a graduated array of rectangular test structures was designed in order to garner a more thorough understanding of the effect of cavitation/RIE on fabricated geometry.

For the this characterization study a graduated array of rectangular structures with designed widths varying from 0.1 um to 5 um by 0.2 um increments was fabricated via the e-beam/RIE/deposition/lift-off process developed for the entrenched WALD NEMS fabrication processes, described in sections 5.5.1 and 5.6.1. The dependence of cavitation/RIE effects on etch time were investigated using two different sample sets. The first set was etched in RIE for 70 seconds, and the second set was etched in RIE for 136 seconds. These etch times were chosen to approximate the designed gate and drain gap heights for the poly-tie devices already described, and are based off of the etch-rates characterized before the system became un-reliable. Fabricated test structures are shown in figures D.1-D.3. In figure D.2
we see that the 0.1 um structure is not fully formed in the structure that was etched for 70 seconds in RIE, but is fully formed in the structure that was etched for 136 seconds. This discovery sheds light on the fabrication limits of the fabrication tools, and limits the geometry of possible designs.

Figure D.1: Structures used for cavitation/RIE characterization. The widths of the rectangular structures were graduated from 0.1-5 um by 0.2 um increments.

After fabrication detailed SEM images were taken of all of the test structures and their dimensions measured using ImageJ. As is evident in figures D.1-D.3 the rectangular structures did not remain rectangular; instead the structures began to merge from the bottom of the gap up, figure D.3. The fabricated width was thus characterized by taking the average of the width of the structure measured at three points: the base, the middle, and the top of the test structure. The average width of each structure was then compared to its designed width and corresponding over-etch widths, and rates calculated. The results of this characterization are shown in figures D.4-D.5.
Figure D.2: Comparison of the narrowest rectangular structures etched in RIE for 70 and 136 seconds before metal deposition/lift-off. Here we see that the 0.1 um structure is not fully formed in the structure that was etched for 70 seconds in RIE, but is fully formed in the structure that was etched for 136 seconds. This discovery sheds light on the fabrication limits of the fabrication tools, and limits the geometry of possible designs.

Figure D.3: SEM images illustrating how the rectangular structures merge as a result of cavitation/RIE

D.1.1 Characterization Results

This characterization study revealed that the average over etch width versus designed width follows a linear trend for both etch times, D.4. The strong linear trend means that
two structures of different widths can be expected to over-etch by proportionally the same amount. Furthermore, this plot shows that the effect of cavitation/RIE is predictable and constant for all time.

Average etch rates for each width were calculated using equation D.1, and are plotted in figure D.5. The linear trend of average etch rate versus designed width is not very strong as it is for over-etch width versus designed width. Because a strong dependence of etch rate on geometry is not readily identifiable, the average etch rate and confidence interval (95% C.I.) was calculated for both time sets, figure D.6. It is obvious from the plot that the two means are identical, and this was verified via Student’s t-test that showed the difference in the two means to be statistically insignificant.

\[ \Delta e = \frac{W_{\text{fabricated}} - W_{\text{designed}}}{2t_{\text{etch}}} \]  

(D.1)

This study was more complete than the first study because a large variety of rectangular geometries were studied. The study revealed limitations of the available fabrication tools, which in turn impose limitations on feasible electrode geometries. Finally, and most importantly, the study was successful in determining an average constant etch-rate that was used to fabricate the gate and drain electrodes with the dimensions specified by the WALD NEMS poly-tie design study already described.

\subsection*{D.1.1.1 Fabrication Results}

Based on the characterization of cavitation/RIE processing effects and the described numerical design studies, WALD NEMS poly-tie inverters/3-terminal switches with entrenched electrodes have been fabricated, and are shown in figure D.7. The dimensions of the fabricated poly-tie WALD NEMS devices are as follows: \( L = 8000 \) nm, \( W_M = 5 \) um, \( W_o = 250 \) nm, \( g_{DS} = 15 \) nm, \( g_{GS} = 65 \) nm and \( D_W = 400 \) nm.

At the time that these first WALD NEMS poly-tie devices were fabricated the RIE
Figure D.4: Average over-etch width Vs. designed width; the data displays an obvious linear trend for both 70 and 136 s etch rates.

Figure D.5: Average over-etch width Vs. designed width; the datum appear to follow a linear trend for both etch times.

remained a tad unstable, even after repairs and the described characterization. This instability was responsible for the overlapping gate and drain electrodes seen in figure D.7, which resulted in gate-to-drain shorting for most of the devices. Furthermore, in this figure sharp features are seen along the anchors. These features were developed because the etch rate...
Figure D.6: Average over-etch rate for structures etched for 70 and 136 s. The difference between the two sets of average over-etch rates for etch times of 70 and 136 s were shown to be statistically insignificant via a student t-test.

Figure D.7: SEM images of 3-terminal Poly-tie switches with overlapping gates and sharp features along the anchors

of SiO$_2$ for the RIE was found to be $\approx 70\%$ of the the previously CNL-characterized rate. Thus the etched trenches were more shallow than they were designed to be. As a result too thick of a layer of metals were deposited, which then resulted in the type of lift-off induced
features that I sought to remove by developing the entrenched processes in the first place! Because of these features many of the fabricated devices were completely fractured at the anchors.

Fortunately, the discrepancy between characterized over-etch rates and actual over-etch rates was slight and could be corrected without requiring another intensive characterization study. Over-etching was completely compensated for by making minor adjustments to the gate electrode and by careful monitoring of the RIE etch rate using via ellipsometry. Over-etched gate electrodes are shown in figure D.8a, and correctly designed/fabricated gate electrodes for WALD NEMS 9th order poly-tie devices are shown in figure D.8b.

![Figure D.8: SEM images of merged gate electrodes, and un-merged gate electrodes. The gate design shown in figure (a) was corrected to compensate for over-etching, figure (b).](image-url)
Appendix E

Secondary MP-FEM Software Details

E.1 Self Consistency

The computational analysis of electromechanical systems requires a self-consistent solution of the coupled interior mechanical domain and the exterior electrostatic domain [138]. This means that computing the electrostatic forces on the un-deformed mechanical domain may not be accurate because deformation of the mechanical structure will cause a redistribution of surface charges, and therefore the electrostatic forces on the deformed structure will differ from those on the un-deformed structure [197].

As an example, and for arguments sake, let us qualitatively model a MEMS/NEMS switch by a 1-D spring mass/parallel plate model. When a potential greater than 0 V is applied to the system, an electrostatic force is generated which causes the device to deform and the gap height to change to some value less than the original. Because a parallel plate model is being considered, the electric field is inversely proportional to the gap height and acts normal to the device surface. If we continue to simulate the actuation of this device in a self-consistent manner, then we will use the updated gap height with some new applied potential to calculate the updated electrostatic load acting on the structure. Again this load will result in an updated displacement. The problem with this model is that information about the curvature of the beam, and thus charge distribution on the surface of the beam, is ignored. Thus all electric fields calculated will be strictly in the y-direction (considering a Cartesian coordinate system), but in actuality the curvature of the deformed structure’s
surface will lead to electric fields with components in the x-direction, which will in turn result in a deformation/deflection not predicted by a simple 1-D model. This can lead to erroneous results, especially for structures which experience significant deformation. Because of this a 1-D quasi-static model does not achieve self consistancy. Thus the deformed mechanical domain must be used to calculate the electric field of the deformed electrostatic domain for a truly self consistent model.

A flow chart illustrating the computational algorithm implemented by the developed software given in appendix F to achieve a self consistent solution is given in figure E.1.

E.2 Mixed Unit System

E.2.1 FEM Model Dimensions

To avoid computational errors in the FEM software a mixed unit system has been implemented. Table E.1 lists physical quantities used by the software, their Si and consistent FEM units, and the physical parameter chosen for the mixed system. For the FEM software it was decided that microns would be used as the fundamental length scale, hence in the table what is meant by consistent FEM units is that the units are all written in terms of µm instead of m. Therefore some quantities in the software are calculated in a µm-s-kg unit system.

<table>
<thead>
<tr>
<th>Physical parameter</th>
<th>Si units</th>
<th>Consistent FEM units</th>
<th>Physical parameter used by FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>l</td>
<td>m</td>
<td>µm</td>
<td>l_{FEM}</td>
</tr>
<tr>
<td>ρ</td>
<td>kg/m^3</td>
<td>kg/µm^3</td>
<td>ρ_{FEM}</td>
</tr>
<tr>
<td>t</td>
<td>s</td>
<td>s</td>
<td>t</td>
</tr>
<tr>
<td>N (force)</td>
<td>kg·m/m^2</td>
<td>kg·s^2/µm^3</td>
<td>N_{FEM}</td>
</tr>
<tr>
<td>V</td>
<td>s^3·A/m^2</td>
<td>s^3·A/µm^2</td>
<td>V_{Si}</td>
</tr>
<tr>
<td>F (capacitance)</td>
<td>m^2·kg/s^2·A^2</td>
<td>m^2·kg/µm^2·A^2</td>
<td>F_{FEM}</td>
</tr>
<tr>
<td>ϵ_o</td>
<td>m^3·kg</td>
<td>m^3·kg</td>
<td>ϵ_{oFEM}</td>
</tr>
</tbody>
</table>
Figure E.1: FEM Model Structure for Self-consistent Solutions
### E.2.2 Conversion Factors: Si to FEM

The following table lists the conversion factors used by the FEM software to convert Si consistent quantities to $\mu m$-$s$-$kg$ quantities.

<table>
<thead>
<tr>
<th>Si Physical Parameter</th>
<th>Conversion Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
<td>$1 \times 10^6$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>$1 \times 10^{-18}$</td>
</tr>
<tr>
<td>$t$ (time)</td>
<td>1</td>
</tr>
<tr>
<td>$N$ (force)</td>
<td>$1 \times 10^6$</td>
</tr>
<tr>
<td>$V$</td>
<td>$1 \times 10^{12}$</td>
</tr>
<tr>
<td>$F$ (capacity)</td>
<td>$1 \times 10^{-12}$</td>
</tr>
<tr>
<td>$A_{132}$</td>
<td>$1 \times 10^6$</td>
</tr>
<tr>
<td>$\epsilon_o$</td>
<td>$1 \times 10^{-18}$</td>
</tr>
</tbody>
</table>
Appendix F

MatLab Code for Multi-physics FEM

Note: Some of the MATLAB files given below call sub-functions from the CALFEM software package. CALFEM is a free FEM software package widely available on the internet.

F.1 MATLAB M-file For Running the Multi-Physics Model

%-----------------------------------------------------------------------
% This software was written by Bradley D. Davidson as part of his PhD
% over the course of nearly 2 years, 2009-2010. The code presented here is
% the most recent version of the code as of July September 2010, we shall
% declare this to be version 1.0, although in acutality this is more like
% version 100.0, but we will discount all of the previous permutations of
% this program as necessary developmental states. The software presented
% here is far from perfect, and is in no way coded efficiently, but the
% code accomplishes what it is intended to do. This is to offer an
% alternative design/analysis tool for NEMS thin film devices, so that the
% engineer/ researcher does not rely on the use of commercial packages such
% as Ansys or Coventor Ware, which gave me such headaches during the
% course of my PhD. In the immortal words of professor K.C. Park,
% "If you want something to work you will have to program it yourself."
%-----------------------------------------------------------------------
% % Model Parameters
% % The following Section is where all inputs for the model are input
% % The inputs include:
% % AnalysisType Type: 2/3-terminal Devices are currently supported
% % Actuation Type: Is the device Gate or Drain Acutated (3-terminal devices)
% % Profile Type: Recangular, Bow-tie, and Poly-Tie profiles are supported
% % Geometry: Source, and electrode geometry
% % Material Properties: Young's Modulus, Density, Poisson's ratio
% % Mesh refinement: Mesh refinement for the source in x and y
% % Time step
% %***********************************************************************

AnalysisType = 10;  % if AnalysisType = 9 ==> Electrostatic solution
                    % if AnalysisType = 10 ==> multiphysics 2 terminal
                    % if AnalysisType = 11 ==> multiphysics 3 terminal
ActuationType = 2;  % if ActuationType = 1 and AnalysisType = 11  
  % ==> drain actuated  
  % if ActuationType = 2 and AnalysisType = 11  
  % ==> gate actuated

InvContact = 0;  % InvContact == 1 for the case the the device is  
  % gate actuated but makes contact with the drain

Profile = 2;  % if Profile = 0 ==> rectangular profile, Wm = Wo.  
  % if Profile = 1 ==> polytie profile (currently 9th order)  
  % if Profile = 2 ==> bowtie profile

Structure = 1;  % if Structure = 0 ==> Cantilever  
  % if Structure = 1 ==> Fixed-fixed Beam

samples = 100;  % This defines the number of sample points

Vstart = 0;  
Voltage = 0;
Vg = 4;
VDD = 0;

if ActuationType == 1
    VAC = Voltage/2*0; %AC amplitude
    % Vg = 0; % for case 11 this is the gate voltage
else
    % Voltage = 0; % for case 11 this is the drain voltage
    VAC = Voltage/2*0; %AC amplitude
end

Fimpulse = 1e3;

%-----------------------------------------------------------------------
% Material properties
%-----------------------------------------------------------------------

E = 400e3; v = 0.28; ro = 19300e-18; % material properties W

%-----------------------------------------------------------------------
% Geometry
%-----------------------------------------------------------------------

fact = 1; % factor can be used for scaling
Wo = fact*.5/2; % minimum device width
Wm = fact*3.5; % maximum device width (for bow/poly-tie devices)
l = fact*3; % length
dw = fact*.25; % drain width
h = 0.032; % thickness of thin film
switch Structure
    case 1
        a = (l-dw)/2;
        b = a+dw;
    otherwise
        a = l - dw;
        b = l;
end

gap_sd = .03; % gap: source to drain
gap_sg = .03; % gap: source to gate

% -----------------------------------
% if Oxides are present on the gate
% gd = 0.15e-9;
% er= 3.8;
% eo = 8.85e-12;
% geff = ((eo*gd + er*(gap_sg-gd)))*1e6/er;
% geff = geff*1e3;
% geff = round(geff)*1e-3;
% -----------------------------------

switch Structure == 1
    case 1 % case for fixed-fixed structures
        if AnalysisType!=11
            gap_gate = gap_sd;
        else
            gap_gate = gap_sg;
        end
    otherwise % case for cantilevers
gap_gate1 = .4; gap_gate2 = gap_sd;
end

% geff = geff*1e3;

%-----------------------------------------------------------------------
% Mesh Refinements in x and y directions
%-----------------------------------------------------------------------

nx = 96; ny = 4;
% nx = 64; ny = 4;

spacing = 1/nx;

lx = 0:spacing:1;

%-----------------------------------------------------------------------
% Shape Functions for the Source Profile
%-----------------------------------------------------------------------

fact = 1;
switch Profile
    case 0 % Rectangular Profile

        Wm = W0;
        [widths lx] = BowTieFunction(lx,W0,Wm,a,b,lx(end),Structure);
    case 1 % Poly-tie Profile

        order = 9; % order of polynomial for fit
        widths = PolyTieFunction(lx*fact,W0*fact,Wm*fact,a*fact,b*fact,...
                                 lx(end)*fact,Structure,order,.75*dw*fact, .75*dw*fact,nx);
case 2  % Bow-Tie Profile

[widths lx] = BowTieFunction( lx, Wo, Wm, a, b, lx(end), Structure);

end

width(:,1) = lx; width(:,2) = widths;  % first column is coordinates,
% 2nd column is widths

%-----------------------------------------------------------------------
% Set up for areas at element centers
%-----------------------------------------------------------------------

for i = 1:length(width)-1;
    meanthick(i,1) = mean([width(i+1,2),width(i,2)]);
end

lel = spacing;
Ael = lel*meanthick;

%-----------------------------------------------------------------------
% clamped BC's
%-----------------------------------------------------------------------

disp_x = 0;  disp_y = 0;  % Fixed in x and y at boundaries

% % Run assembly code
% 
% % The Function called here calculates:
% % The Global Stiffness Matrices K and M
% All information about node points of the mesh
%

%************************************************************************

[K M fecoord, fetopo, feprop, febc, numfenod, numfele, edof, Ex, Ey, ep, D] = ... 
    AssembleKM(E, v, ro, width, 0, 1, h, nx, ny);

%------------------------------------------------------------------------

% Nodal Location for center displacement
%------------------------------------------------------------------------

switch Structure % We need to know the location of the point of maximum
    % deflection so that we can analyze pull-in voltages
    %
    case 1 % Maximum deflection at the center of the beam
        loc = find(fecoord(:, 1) == l/2);
            loc = 2*loc(1);
    case 0 % maximum deflection at the tip of the beam
        loc = find(fecoord(:, 1) == l);
            loc = 2*loc(1);
end

% assign boundary conditions/flags
%************************************************************************

j = 1;
for i = 1:length(febc)
    if febc(i, 1) == 3;
        bc(j:j+1,:) = [2*i-1 disp_x; 2*i disp_y];
            j = j+2;
    end
j = 1;
for i = 1:length(febc)
    if febc(i,1) == 2;
        flagu(j:j+1,:) = [2*i-1;2*i];
        j = j+2;
    end
end
end

j = 1;
for i = 1:length(febc)
    if febc(i,1) == 2;
        nls(j,:) = i;
        j = j+1;
    end
end
end

%% eigen frequencies, used for vibration analysis only
%************************************************************************

[Eig,EigVect]=eigens(K,M,bc(:,1),1);
freq = sqrt(Eig);

%% Setup Times steps
%************************************************************************

switch ActuationType
    case 1
        tstart = round(Vstart/Voltage*100)/100;
    case 2
        tstart = round(Vstart/Vg*100)/100;
end
end

switch AnalysisType
    case {2,7,10,11}
        tend = 1; % for use in the linear loading case
        steps = samples;
        tstep = tend/steps;
        t = tstart:tstep:tend;
    otherwise
        tend = samples*2*pi/freq; % for use with frequency Analysis
        tstep = (1/10)*2*pi/freq;
        t = 0:tstep:tend;
end

% dsamp = length(t)/(tend-t(1));
% save Samp.mat dsamp

%% NonLinear Newmark Solver
%********************************************************************>

beta = .25; % Newmark Parameters
gamma = .5;

extents = [a b 0 (gap.gate-gap.sd) gap.gate]; % electrostatic domain

Vgs = t*Voltage;

[U V A t forcehistory ekinhistory epothistory events]...
= NonLinearNewmarkSolver(beta, gamma, t, tstep, febc, Voltage, VAC, Vg, ...
VDD, freq, width, Ael, gap_sd, extents, loc, AnalysisType, ActuationType, ...
bc, flagu, edof, Ex, Ey, numfele, numfenod, fecoord, nls, Fimpulse, spacing, ...
l, nx, ep, D, ro, Wo, Wm, dw, Structure, InvContact, Profile);

U = full(U);

%% for Tunneling analysis/ Export for Excel
dlmwrite('femUV2t.101710.dat',U)
% Vgs = t*Vg;
%
save femUV2t.1017.mat U Vgs

% save Signal.mat  U V A t forcehistory events ekkinhistory epothistory...
% Voltage Vg VAC AnalysisType;

%% pulliin
% This function extracts the pull-in voltage for the analysis
%************************************************************************
pi = Pullin_MP(U, t, Voltage, Vg, AnalysisType, ActuationType,...
    [a b 0 (gap_gate-gap_sd) gap_gate], InvContact);

disp(['Pullin Voltage: ' num2str(pi) ' V'])

%% Plotting
%
% Here the Poincare (phase diagrams), and displacement Vs. voltage etc
% plots are generated
%************************************************************************
y = PoincarePlotsMP(U,V,A,t,forcehistory, ekinhistory, epothistory,...
    events, Voltage, Vg,Vg,VAC,AnalysisType,ActuationType);

F.2 Numerical Solvers

F.2.1 Non-Linear Newmark Solver

function [U V A t forcehistory ekinhistory epothistory events]...
    = NonLinearNewmarkSolver(beta, gamma, t, tstep, febc,...
        Voltage, VAC, Vg, VDD, freq, thick, Area, gap, sd, extents, loc,...
        AnalysisType, ActuationType, bc, flagu, edof, Ex, Ey, numfele, numfenod,...
        fecoord, nls, Fimpulse, spacing, l, nx, ep, D, ro, Wo, Wm, dw, DeviceType,...
        InvContact, Profile)

%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% %
% % This function uses the Non-linear Newmark solver to solve for device
% % displacements for a given load
% %
% %-----------------------------------------------------------------------

% Allocating some memory

f = sparse(2*numfenod,1);
U = sparse(2*numfenod,2); % Initializing f, U, V, A
V = sparse(2*numfenod,2);
A = sparse(2*numfenod,2);

% Free degrees of freedom (meaning no boundary conditions)
\text{nd} = 2 \times \text{numfenod};
\text{fdof} = [1:nd]';
\text{pdof} = \text{bc}(:,1); \quad \% \text{nodes that have bcs}
\text{dp} = \text{bc}(:,2);
\text{fdof}(\text{pdof}) = []; \quad \% \text{free nodes}

\% \text{set up 'velocity' impulse for frequency analysis}

\text{switch} \ \text{AnalysisType}
\begin{align*}
\text{case} \ \{3, 8, 9\} \\
V(\text{fdof},1) &= -\text{Fimpulse}; \\
V(\text{pdof},1) &= \text{dp}; \\
i &= 1:2:\text{length}(V); \quad \% \text{need to set horizontal displacements to zero} \\
V(i,:) &= 0;
\end{align*}
\text{end}

\% \text{Begin Simulation}

\text{displacement}(1,1) = \text{U}(\text{loc},1); \% \text{I.C.s at the point of maximum deflection}
\text{velocity}(1,1) = V(\text{loc},1);
\text{acceleration}(1,1) = A(\text{loc},1);

\text{for} \ i = 1:\text{length}(t)
\begin{align*}
\text{disp(['timestep: ' num2str(i) ' of ' num2str(length(t))])} \\
\text{timestep} &= i; \\
\% \text{---------------------------------------------------------------------------------------------------------------------} \\
\% \text{Predictor/ Corrector values for newmark method} \\
\text{U}(::2) &= \text{U}(::1) + \text{tstep} \times V(::1) + (0.5 - \text{beta}) \times \text{tstep}^2 \times A(::1); \\
\text{U}(\text{pdof},2) &= \text{dp};
\end{align*}
\text{end}
\begin{verbatim}
V(:,2) = V(:,1) + (1-gamma) * tstep * A(:,1);
V(pdof,2) = dp;
A(pdof,2) = dp;

%-------------------------------------------------------------------->

Un = U(:,2);
Vn = V(:,2);
An = A(:,2);

Uc = CenterDisplacements(Un,nls);  \% displacement at the elem. centers

%% Attempt at getting the forces from the electric field

\textbf{switch} AnalysisType

\textbf{case} 10  \% Two-Terminal Multi-Physics

[Efx Efy] = ElectroStatic2t_V2(l,nx,nls,Un(flagu),...
gap_sd,Voltage,t(i));

[Cap(i,:) = Capacitance2t(Area,Uc,nls,gap_sd);
[Q(i,:]) = Charge2t(Cap(i,:), Voltage, t(i));
[f] = ElectroStaticForce(Q(i,:), Efx, Efy, flagu,numfenod);

\textbf{case} 11  \% Three-Terminal Multi-Physics

[Efx Efy] = ElectroStatic3t(l,nx,nls,Un,extents,Voltage,Vg,...
VDD,t(i), AnalysisType,ActuationType,...
InvContact,timestep);  \% calculate e-field
\end{verbatim}
\[ \text{Cap}(i,:) \] \text{gl}_el \text{ d}_el \text{ gr}_el \] = Capacitance3t(Un,nls,fecoord,...
   extents,Wo,Wm,DeviceType,Profile); \% calculate capacitance

\[ Q(i,:) \] = Charge3t(Cap(i,:), Voltage,Vg,VDD,fecoord,...
   extents,nls,t(i),ActuationType,...
   \text{gl}_el,\text{ d}_el,\text{ gr}_el); \% calculate charge

\[ f \] = ElectroStaticForce(Q(i,:), Efx, Efy, flagu,numfenod);

\textbf{otherwise} \% Mechanical Models with approximated electrostatic loads
\[ f \] = Loads_EVC(Voltage,VAC,freq,thick,Area,gap_sd,t(i),Uc,...
   febc,f,AnalysisType,nls,Fimpulse,spacing,1);

end

\% Electrostatic softening (Used for approximated loading Cases

\textbf{switch} AnalysisType
   \textbf{case} \{6,7\}
      Kelectric = ElectricStiffness(AnalysisType,Area,Voltage,...
         gap_sd,numfenod,t(i),nls,Uc,VAC,freq);
   \textbf{otherwise}
      Kelectric = 0; \% just a place holder
end

\% Calculate the Residual

\[ [R \ Kt \ f1] \] = Res(U(1:2),V(1:2),A(1:2),f,f dof,Ex, Ey,numfele,numfenod,...
   edof,ep,D,ro,t step,b eta,AnalysisType,Kelectric);
ref = max(norm(fi(fdof)),norm(R(fdof))); % the inner Newton loop of the Newmark Solver

maxiter = 30;
iter = 0;
relref = .9;
neweps = 1e-7;
newrlx = 1;

while relref > neweps && iter < maxiter
    [R Kt fi ekin epot] = Res(Un,Vn,An,f,fdof,Ex,Ey,numfele,...
        numfenod,edof,ep,D,ro,tstep,beta,AnalysisType,Kelectric);
    relref = norm(R(fdof))/ref; % convergence check
    Delta u = -Kt(fdof,fdof)\R(fdof); % u increment
    Un(fdof) = Un(fdof)+newrlx*Delta u; % Update displacements
    Vn(fdof) = Vn(fdof)+...
        gamma/beta/tstep*newrlx*Delta u; % update velocities
    An(fdof) = An(fdof)+...
        1/beta/tstep^2*newrlx*Delta u; % update accelerations
    iter = iter+1;
end

if iter >= maxiter
    disp(['Newton did not Converge, relref = ' num2str(relref)])
else
    disp(['Newton Converged, relref = ' num2str(relref)])...
at iteration ' num2str(iter) ]);
end

%% Juggle and store U, V, A to begin next time step

U(:,2) = Un;
V(:,2) = Vn;
A(:,2) = An;

U(:,1) = U(:,2);
V(:,1) = V(:,2);
A(:,1) = A(:,2);

%% Storage purposes

displacement(i,1) = U(loc,1);
velocity(i,1) = V(loc,1);
acceleration(i,1) = A(loc,1);
forcehistory(i,1) = f(loc,1);
ekinhistory(i,1) = ekin;
epothistory(i,1) = epot;

%% cases for exiting the analysis
switch AnalysisType

case {2,6,7,8,9}

    events(i,:) = det((5+1e-1)*Kt(fdof,fdof)/(max(max(Kt(fdof,fdof)))

otherwise

    events = [i,1];
end
if AnalysisType == 2 && abs(displacement(i,1)) > 2*gap.sd/3
    break
end

if AnalysisType == 6 && sign(events(i,1)) < 0
    break
end

if AnalysisType == 7 && sign(events(i,1)) < 0
    break
end

if AnalysisType == 9 && sign(events(i,1)) < 0
    break
end

if AnalysisType == 10 && abs(displacement(i,1)) > ...
    (extents(5)-extents(4))
    break
end

switch InvContact
    case 0

        if AnalysisType == 11 && abs(displacement(i,1)) > .9*extents(5)
            break
        end

otherwise

        if AnalysisType == 11 && abs(displacement(i,1)) ≥ ...
            (extents(5)-extents(4))
        end
if displacement(i,1) > 0
    break
end

events = 1;

end

t = t(1:i);
U = displacement;
V = velocity;
A = acceleration;

F.2.2 Electric Field Solver for a 3-terminal Device

function [Efx Efy] = ElectroStatic3t(l,nx,nls,disp,extents,...
    Voltagedrain,Voltagegate,VDD,t, AnalysisType,...
    ActuationType,InvContact,timestep)

%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% % This function solves for the Electric field for 3-terminal devices
% % load fortesting.mat

%-----------------------------------------------------------------------
% t = t(1)
%% define the electrostatic domain

xmin = 0;  xmax = l;  l = xmax-xmin;
ymin = 0;  ymax = extents(5);  h = ymax-ymin;

n = 8;  % number of mechanical elements for electrical element

nxref = nx/n;  % number of divisions in x
nyref = extents(5)/(.01/5);  % number of divisions in y
elx = l/nxref;  % number of elements in x
ely = h/nyref;  % number of elements in y

E = 10e10;  % these are properties of the electrostatic
v = 0;  % domain representative material
ro = 1e0;
thick = 1;

%% get the nodal displacements which correspond to the coarse mesh nodes
% Here we finding the displacements from the mechanical model that
% correspond to the electrostatic domains mesh points

nodes = 1:1:nls(end)*2;

k = 1;
for i = 1:2*n:length(nodes)
    nodesC(k,1) = nodes(i);
    nodesC(k+1,1) = nodesC(k,1)+1;
    k = k+2;
disp = disp(nodesC);

%% deformed electrostatic domain

% get a faux stiffness matrix for a lagrangian description
[K, fecoord, fetopo, feprop, febc, numfenod, numfele, edof, Ex, Ey, ep, D]...
= Assemble_K_Efield(E, v, ro, thick, i, h, nxref, nyref, 0);

% we need to find the nodal points where the drain resides and restrict
% their movement (add boundary conditions)

% save test4drainbc.mat fecoord febc extents elx ely nxref nyref
if ActuationType == 1 || InvContact == 1
    febc = DrainBcs(fecoord, febc, extents, elx, ely, nxref, nyref);
end

% assign boundary conditions for mechanics

j = 1;
k = 1;
for i = 1:length(febc)
    if febc(i,1) == 3;
        bc(j:j+1,:) = [2*i-1 0;2*i 0];
        j = j+2;
    elseif febc(i,1) == 2
        bc(j:j+1,:) = [2*i-1 disp(k);2*i disp(k+1)];
        k = k+1;
    end
end
j = j+2;
k = k+2;
end
end

j = 1;
for i = 1:length(febc)
    if febc(i,1) == 2
        flagdisp(j:j+1,:) = [2*i-1 disp(j);2*i disp(j+1)];
j = j+2;
    end
end

flagd = flagdisp(:,1);

nd = 2*numfenod;
fdo =[1:nd]';
% Start with all degrees of freedom free
pdo = bc(:,1);
% Nodes that have conditions
dp = bc(:,2);
% Assigned Displacements
fdo(pdo) = [];
% Remove the fixed node numbers from the free node set

%-----------------------------------------------------------------------

% Solve for the deformed mesh
%-----------------------------------------------------------------------

fext = zeros(nd,1);
% zero applied load
u = zeros(nd,1);
% Initialize the displacement vector
u(flagd) = flagdisp(:,2);

Kpart = K;
% partitioned K for prescribed conditions
Kpart(pdo,:) = [];
% Kpart has the prescribed rows and columns removed
fpart = -Kpart(:,pdof)*bc(:,2); % solve for the forces imparted by
% prescribed conditions

u(fdof) = K(fdof,fdof)part; % Use the forces to solve for the
% displacements at the free nodes.

%Plot Deformed Mesh
% figure(10)
% disp = u;
% ed=extract(edof,disp);
% xlim([0 8])
% eldisp2(Ex,Ey*100,ed,[2 2 0],10);
% grid on

%% back to the electrostatics....
[coord] = ElectricFieldCoords_v2(fecoord,u);

switch AnalysisType
 case 11

  % add the coordinates of the drain
  save test4drain.mat extents coord ely h elx nxref nyref u
  [coord gridx gridy spacing nelements gradcoord WD cmidx] ...
  = DrainFieldCoords(extents, coord, elx, ely, h,nxref,nyref,u);

  if timestep == 1; % these steps only need to be done once because
    % they are constant in time
% finds the drain coordinates
save test4sorter.mat coord spacing ely extents elx u
[draincoord, draincoordl, draincoordr, draincoordt] = DrainSorter_3T(coord, spacing(2, 2), ely, extents, u, WD, cmidx);

% transform nodal coordinates to row and column space
[draingrid, dglbc, dgrbc, dgtbc, dginterior] = Drainmeshlocations_3t(nelements+nxref, nyref, draincoord, draincoordl, draincoordr, draincoordt, spacing, elx, ely, gradcoord);
save draingridlocations.mat draingrid dglbc dgrbc dgtbc dginterior
end

otherwise
[draincoord, draincoordl, draincoordr, draincoordt] = DrainSorter(coord, elx, ely, extents);

[draingrid, dglbc, dgrbc, dgtbc, dginterior] = Drainmeshlocations(nxref, nyref, draincoord, draincoordl, draincoordr, draincoordt, elx, ely);
end

% **PLEASE NOTE, DGLBC IS NOW THE COORDINATES FOR THE PART OF THE DRAIN THAT
% SHOULD HAVE THE SAME DIRCHLET ENFORCEMENT CONDITIONS FOR THE BOUNDARY
% WITH A RIGHT FACING NORMAL. THUS THE DGRBC HAS THE BOUNDARY FOR THE LEFT
% FACING NORMAL**

% % Solve The Laplace equation for the Electrostatic Domain
\texttt{Bcs = zeros(nxref+1,4); \hspace{1cm} \% Boundary Potentials}
\texttt{Bcs(:,1) = VDD;}
\texttt{if ActuationType == 1}
\texttt{\hspace{2cm} Bcs(:,2) = Voltagegate;}
\texttt{\hspace{2cm} Bcsdrain = Voltagedrain*t;}
\texttt{elseif ActuationType == 2}
\texttt{\hspace{2cm} Bcs(:,2) = Voltagegate*t;}
\texttt{\hspace{2cm} Bcsdrain = Voltagedrain;}
\texttt{elseif ActuationType == 3}
\texttt{\hspace{2cm} Bcs(:,2) = Voltagegate*t;}
\texttt{\hspace{2cm} Bcsdrain = Voltagedrain*t;}
\texttt{end}

\texttt{if AnalysisType ==11}
\texttt{\hspace{1cm} \% laplace solver}
\texttt{\hspace{1cm} \[potential rx ry iterations error\]= LaplaceSolver3t(Bcs,Bcsdrain,coord,draingrid,dglbc, dgrbc, ...}
\texttt{\hspace{1cm} \hspace{2cm} dgtbc,dginterior, nxref+nelements,nyref,ActuationType);} 
\texttt{\[fx fy\] = Gradient_3TV2(potential,rx,ry,coord,dglbc,dgrbc,dgtbc, ...}
\texttt{\hspace{2cm} \hspace{2cm} nxref+nelements,nyref);} 
\texttt{else}
\texttt{\hspace{1cm} \[potential rx ry iterations error\]= LaplaceSolver3t(Bcs,Bcsdrain,coord,draingrid,dglbc,dgrbc, ...}
\texttt{\hspace{2cm} \hspace{2cm} dgtbc,dginterior, nxref,nyref);}
\[ [fx \ fy] = \text{Gradient3t(potential,rx,ry,coord,dglbc,...
  dgrbc,dgtbc,nxref,nyref)]; \]

end

%% The Electric field is -grad(Potential)

Efx = -fx;
Efy = -fy;

%% plotting of the field

% if AnalysisType ==11
%   ll = nelements(1)+nxref+1;
%   for i = 1:nyref+1
%     X(i,:) = coord((i-1)*ll+1:i*ll,1);
%   end
%   for i=nyref+1:-1:1
%     Y(i,:) = coord((i-1)*ll+1:i*ll,2);
%   end
%   [a b] = size(Y);
%   dummy = zeros(a,b);
%   for i = 1:a
%     dummy(a+1-i,:) = Y(i,:);
%   end
%   scale = 100;
%   Y = scale*dummy;
for i = 1:nxref+1
    X(i,:) = coord((1+(i-1)*length(gridpoints)):(i-1)*...length(gridpoints))+length(gridpoints),1);
    Y(i,:) = coord((1+(i-1)*length(gridpoints)):(i-1)*...length(gridpoints))+length(gridpoints),2);
end
end

% % Plot the Potential and the Electric Field
% figure(2)
% contourf(X,Y,potential)
% colorbar
% hold on
% quiver(X,Y,Efx,Efy)
% grid on
%
% % Plot the Potential surface
% figure(11)
% surf(X,Y,potential)
% colorbar
% grid on
%
% E-field (FL Electric Mesh to Mechanical Domain

[Ef y Efx] = LoadDistribution3T(1,nx,gridx,Efy,Efx);

F.2.3 Electric Field Solver for a 2-Terminal Device
function [Efx Efyl] = ElectroStatic2t_V2(l,nx,nls,disp,gap,Voltage,t)

%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% This function solves for the Electric field for 2-terminal devices
%-----------------------------------------------------------------------

xmin = 0; xmax = l; l = xmax-xmin;

ymin = 0; ymax = gap; h = ymax-ymin;

n = 4;

nxef = nx/n; % number of electrostatic elements, must be nx/8;

nyef = nxef;

gridx = (0:l/nxef:l)';

% faux chosen material properties for the deformable domain
E = 10e10;
v = .5;
ro = 1e0;
thick = 1;

% get the nodal displacements which correspond to the coarse mesh nodes
nodes = 1:1:nls(end)*2;
k =1;
for i = 1:2*n:length(nodes)
    nodesC(k,1) = nodes(i);
    nodesC(k+1,1) = nodesC(k,1)+1;
    k = k+2;
end

disp = disp(nodesC);

% get the nodal displacements which correspond to the coarse mesh nodes
nodes = 1:1:nls(end)*2;
k =1;
for i = 1:2*n:length(nodes)
    nodesC(k,1) = nodes(i);
    nodesC(k+1,1) = nodesC(k,1)+1;
    k = k+2;
end

disp = disp(nodesC);

% get a faux stiffness matrix for a lagrangian description
[K,feoord,fetopo,feprop,febc,numfenod,numfele,edof,Ex,Ey,ep,D]...
% assign boundary conditions for mechanics
j = 1;
k = 1;
for i = 1:length(febc)
    if febc(i,1) == 3;
        bc(j:j+1,:) = [2*i-1 0;2*i 0];
        j = j+2;
    elseif febc(i,1) == 2
        bc(j:j+1,:) = [2*i-1 disp(k);2*i disp(k+1)];
        j = j+2;
        k = k+2;
    end
end
end
j = 1;
for i = 1:length(febc)
    if febc(i,1) == 2
        flagdisp(j:j+1,:) = [2*i-1 disp(j);2*i disp(j+1)];
        j = j+2;
    end
end
flagd = flagdisp(:,1);

nd = 2*numfenod;
fdo=1:nd;'
pdo= bc(:,1);
dp=bc(:,2);
fdo(pdo)=[];

%% Solve for the deformed mesh
fext = zeros(nd,1);
u = zeros(nd,1);
u(flagd) = flagdisp(:,2);

Kpart = K;
Kpart(pdof,:) = [];
fpart = -Kpart(:,pdof)*bc(:,2);
u(fdof) = K(fdof,fdof)
fpart;

% Plot Deformed Mesh
% figure(4)
% disp = u;
% ed = extract(edof,disp);
% eldisp2(Ex,100*Ey,ed,[2 2 0],100);
% grid on

%% back to the electrostatics....
Bcs = zeros(nxef+1,4);
Bcs(:,1) = 0;
Bcs(:,2) = Voltage*t;

[coord gridpoints]...
    = ElectricFieldCoords(fecoord,disp,xmin,xmax,ymin,ymax,nxef,nyef);

[potential rx ry iterations error] = LaplaceSolver2t(Bcs,coord,nxef,nyef);

[fx fy] = Gradient2t(potential,rx,ry,coord,nxef,nyef);

%% The Electric field is -grad(Potential)
Efx = -fx;
Efy = -fy;

% extract the electric field at the source
% for i = 1:nyef+1
  X(i,:) = coord((1+(i-1)*length(gridpoints)):(i-1)*...
             length(gridpoints))+length(gridpoints),1);
  Y(i,:) = coord((1+(i-1)*length(gridpoints)):(i-1)*...
             length(gridpoints))+length(gridpoints),2);
 end

% Plot the Potential and the Electric Field
% figure(2)
% contourf(X,Y,potential)
% colorbar
% hold on
% quiver(X,Y,Efx,Efy)
% grid on
%
% % Plot the Potential surface
% figure(3)
% surf(X,Y,potential)
% colorbar
% grid on

% number of nodes for the source, ratio must be 8:1 for interpolation

% E-field (FL Electric Mesh to Mechanical Domain

[Efy Efx] = LoadDistribution3T(1,nx,gridx,Efy,Efx);

F.2.4 Laplace Solver for 3-Terminal Electrostatic Domains
function [potential rx ry iter err]...
    = LaplaceSolver3t_V2(Bcs,Bcsdrain,coord,draingrid,dglbc,...
                     dgrbc, dgtbc,dginterior, nx,ny,SubCase)

%%-----------------------------------------------------------------------
% This program will compute the potential between deformed plates for
% my NEMS devices
% inputs: Bcs = boundary conditions
% disp = displacement vector for the deforemed beam's nodal points
% Outputs: potential is the matrix of the potential values
%%-----------------------------------------------------------------------

% *****PLEASE NOTE, DGLBC IS NOW THE COORDINATES FOR THE PART OF THE DRAIN
% THAT SHOULD AHVE THE SAME DIRCHLET ENFORCEMENT CONDITIONS FOR THE BOUNDARY
% WITH A RIGHT FACING NORMAL. THUS THE DGRBC HAS THE BOUNDARY FOR THE LEFT
% FACING NORMAL*****

nx = round(mean(nx));

for i = 1:4
    guess(i) = mean(Bcs(:,i));
end

if sum(guess) \neq 0
    guess = mean(guess)*ones(ny+1,nx+1);
else
    guess = mean(Bcsdrain)*ones(ny+1,nx+1)/4;
end
mesh = zeros(size(guess));

guess(:,1) = Bcs(1,3);
guess(:,end) = Bcs(1,4);
guess(1,:) = Bcs(1,1);

% if SubCase == 2
guess(end,:) = Bcs(1,2);
guess(dgtbc(1,1),dgtbc(1:length(dgtbc),2)) = Bcsdrain;
% end

for i = 1:length(dginterior)
    guess(dginterior(i,1),dginterior(i,2)) = 0;
end

mesh = guess;

rx = zeros(size(mesh));
ry = zeros(size(rx));

%%% x-direction radii

for i = 1:ny+1 % Interior radii
    for j = 2:nx
        ele = (i-1)*(nx+1)+j;
        rx(i,j) = (sqrt((coord(ele,1)-coord(ele-1,1))^2+...)
            (coord(ele,2)-coord(ele-1,2))^2)...
            +sqrt((coord(ele,1)-coord(ele+1,1))^2+...
(coord(ele,2)-coord(ele+1,2))^2)/2;

end
end

% for dirchlet bcs on the left side

for i = 1:ny+1
    j = 1;
    ele = (i-1)*(nx+1)+j;
    rx(i,j) =sqrt((coord(ele,1)-coord(ele+1,1))^2+...
    (coord(ele,2)-coord(ele+1,2))^2);
end

% for dirchlet bcs on the right side

for i = 1:ny+1
    j = nx+1;
    ele = (i-1)*(nx+1)+j;
    rx(i,j) =sqrt((coord(ele,1)-coord(ele-1,1))^2+...
    (coord(ele,2)-coord(ele-1,2))^2);
end

%% y-direction radii

for i = 2:ny
    for j = 1:nx+1
        ele = (i-1)*(nx+1)+j;
        ry(i,j) = (sqrt((coord(ele,1)-coord(ele-(nx+1),1))^2+...
        (coord(ele,2)-coord(ele-(nx+1),2))^2)... +sqrt((coord(ele,1)-coord(ele+(nx+1),1))^2+...
        (coord(ele,2)-coord(ele+(nx+1),2))^2))/2;
    end
end
% for dirchlet bcs on the top

for j = 1:nx+1
    i = 1;
    ele = (i-1)*(nx+1)+j;
    ry(i,j) = \sqrt{((\text{coord}(ele,1)-\text{coord}(ele+(nx+1),1))^2+...}
              \((\text{coord}(ele,2)-\text{coord}(ele+(nx+1),2))^2)};
end

% for dirchlet bcs on the right side

for j = 1:nx+1
    i = ny+1;
    ele = (i-1)*(nx+1)+j;
    ry(i,j) = \sqrt{((\text{coord}(ele,1)-\text{coord}(ele-(nx+1),1))^2+...}
              \((\text{coord}(ele,2)-\text{coord}(ele-(nx+1),2))^2)};
end

dummy = zeros(ny+1,nx+1);
for i = 1:ny+1
    dummy(ny+2-i,:) = ry(i,:);
end

ry = dummy;

%% iterations

err = 1e3;
iter = 1;

%% potential on sides with dirchlet conditions imposed
while err > 1e-15

%% All dirchlet like conditions
if SubCase == 1
    for i = 2:ny % Potential of left/right side with Dirchlet
        j = [1 nx+1];
        mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
        mesh(ny+1,j) = 1/(2)*(guess(i-1,j)+guess(i,j));
    end
elseif SubCase == 2
    for i = 2:ny % Potential of left and right side with Dirchlet
        j = [1 nx+1];
        mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
    end
end

% this loop will take care of the electrically isolated area between % drain and gate electrodes
if SubCase == 1
    for i = dgtbc(1,1)+1:ny %interior for rows
        for j = [dglbc(1,2) dgrbc(1,2)] % first and last column
            mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
            mesh(ny+1,j) = 1/(2)*(guess(i-1,j)+guess(i,j));
        end
    end
elseif SubCase == 2
    for i = dgtbc(1,1)+1:ny %interior for rows
        for j = [dglbc(1,2) dgrbc(1,2)] % first and last column
            mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
        end
    end
if SubCase == 1
    % gate bottom has dirchlet like conditions

    for i = ny+1
        % Potential of left and right side gate with Dirchlet
        j = 2:dglbc(1,2);
        mesh(i,j) = 1/(2)*(guess(i,j-1)+guess(i,j+1));
    end

    for i = ny+1
        j = dgrbc(1,2):nx;
        mesh(i,j) = 1/(2)*(guess(i,j-1)+guess(i,j+1));
    end

elseif SubCase == 2
    % dirchlet like conditions on the drain

    for i = dgtbc(1,1)
        % Potential of left/right gate with Dirchlet
        j = dglbc(1,2):dgrbc(1,2);
        mesh(i,j) = 1/(2)*(guess(i,j-1)+guess(i,j+1));
    end

dj

end

%% potential of interior

for i = 2:dgtbc(1,1)-1
    for j = 2:nx
        mesh(i,j) = 1/(2*(rx(i,j)^2+ry(i,j)^2))*(ry(i,j)^2*(guess(i,j+1)+guess(i,j-1))+rx(i,j)^2*...*(guess(i,j+1)+guess(i,j-1))+rx(i,j)^2*...
for i = dgtbc(1,1):ny
    for j = 2:dglbc(1,2)-1
        mesh(i,j) = 1/(2*(rx(i,j)^2+ry(i,j)^2))*ry(i,j)^2*(
            (guess(i,j+1)+guess(i,j-1))... 
            +rx(i,j)^2*(guess(i-1,j)+guess(i+1,j)));
    end
end

for i = dgtbc(1,1):ny
    for j = dgrbc(1,2)+1:nx
        mesh(i,j) = 1/(2*(rx(i,j)^2+ry(i,j)^2))*ry(i,j)^2*(
            (guess(i,j+1)+guess(i,j-1))... 
            +rx(i,j)^2*(guess(i-1,j)+guess(i+1,j)));
    end
end

for i = 1:length(dginterior)
    mesh(dginterior(i,1),dginterior(i,2)) = 0;
end

err = norm(mesh-guess);
guess = mesh;

if iter > 5e3
    potential = mesh;
    return
end
F.2.5 Laplace Solver for 2-Terminal Electrostatic Domains

```matlab
function [potential rx ry iter err] = LaplaceSolver2t(Bcs,coord,nx,ny)

%%-----------------------------------------------------------------------
% This program will compute the potential between deformed plates
% Outputs: potential is the matrix of the potential values
%%-----------------------------------------------------------------------

for i = 1:4
    guess(i) = mean(Bcs(:,i));
end

for i = 1:4
    guess(i) = mean(Bcs(:,i));
end

mesh = zeros(size(guess));
guess(1,:) = Bcs(:,1)';
guess(end,:) = Bcs(:,2)';
guess = mean(guess)*ones(nx+1,ny+1);

for i = ny+1:-1:1
    ele = (i-1)*(nx+1)+j
    rx(i,j) = (sqrt((coord(ele,1)-coord(ele-1,1))^2+...
```
(coord(ele,2)-coord(ele-1,2))^2)+...

sqrt((coord(ele,1)-coord(ele+1,1))^2+... 
(coord(ele,2)-coord(ele+1,2))^2))/2;

end
end

% for dirchlet bcs on the left side
for i = ny+1:-1:1 
    j = 1;
    ele = (i-1)*(nx+1)+j;
    rx(i,j) =sqrt((coord(ele,1)-coord(ele+1,1))^2+... 
                  (coord(ele,2)-coord(ele+1,2))^2));
end

% for dirchlet bcs on the right side
for i = ny+1:-1:1 
    j = nx+1;
    ele = (i-1)*(nx+1)+j;
    rx(i,j) =sqrt((coord(ele,1)-coord(ele-1,1))^2+... 
                  (coord(ele,2)-coord(ele-1,2))^2));
end

%%% y-direction radii
for i = ny:-1:2 
    for j = 1:nx+1 
        ele = (i-1)*(nx+1)+j;
        ry(i,j) = (sqrt((coord(ele,1)-coord(ele-(nx+1),1))^2+...
                        (coord(ele,2)-coord(ele-(nx+1),2))^2))...
                  +sqrt((coord(ele,1)-coord(ele+(nx+1),1))^2+...
                        (coord(ele,2)-coord(ele+(nx+1),2))^2))/2;
    end
end
% for dirchlet bcs on the top
for j = 1:nx+1
    i = 1;
    ele = (i-1)*(nx+1)+j;
    ry(i,j) = sqrt((coord(ele,1)-coord(ele+(nx+1),1))^2+... 
                  (coord(ele,2)-coord(ele+(nx+1),2))^2);
end

% for dirchlet bcs on the right side
for j = 1:nx+1
    i = ny+1;
    ele = (i-1)*(nx+1)+j;
    ry(i,j) = sqrt((coord(ele,1)-coord(ele-(nx+1),1))^2+... 
                  (coord(ele,2)-coord(ele-(nx+1),2))^2);
end
dummy = zeros(ny+1,nx+1);
for i = 1:ny+1
    dummy(ny+2-i,:) = ry(i,:);
end
ry = dummy;

%% iterations
err = 1e3;
iter = 1;

while err > 1e-6   % Convergence Criteria
    for i = 2:ny   % Potential of left side with Dirchlet conditions imposed
        j = 1;
        mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
    end
end

for i = 2:ny
    % Potential of right side with Dirichlet conditions imposed
    j = nx+1;
    mesh(i,j) = 1/(2)*(guess(i-1,j)+guess(i+1,j));
end

for i = 2:ny
    % Potential of interior
    for j = 2:nx
        mesh(i,j) = 1/(2*(rx(i,j)^2+ry(i,j)^2))*(ry(i,j)^2*(guess(i,j+1)+guess(i,j-1)) + rx(i,j)^2*(guess(i-1,j)+guess(i+1,j)));
    end
end

err = norm(mesh-guess);
guess = mesh;
if iter > 5e3
    potential = mesh;
    return
end
iter = iter+1;
end

potential = mesh;

\subsection{Bow-tie Shaped Structures}

\begin{verbatim}
function [width lx] = BowTieFunction(x,Wo,Wm,a,b,l,DeviceType)

%-----------------------------------------------
\end{verbatim}
switch DeviceType
    case 1
        y = zeros(length(x),1);
        flag = find(x == a);
        if sum(flag) == 0;
            x(end+1:end+2) = [a b];
            y = zeros(length(x),1);
        end
        x = sort(x);
        flag = find(x == a);
        y(1:flag,1) = (Wo-Wm)/a*x(1:flag)+Wm;
        flag2 = find(x == b);
        y(flag+1:flag2,1) = Wo;
        y(flag2+1:end) = (Wm-Wo)/(l-b)*x(flag2+1:end)-(Wm-Wo)/(l-b)*b+Wo;
otherwise

\[
y = \text{zeros}(\text{length}(x),1);
\]

\[
\text{flag} = \text{find}(x == a);
y(1:flag,1) = (Wo-Wm)/a \times x(1:flag)+Wm;
\]

\[
\text{flag2} = \text{find}(x == b);
y(\text{flag}+1:\text{flag2},1) = Wo;
\]

\[
y(\text{flag2}+1:\text{end}) = Wo;
\]

end

width = 2*y;
lx = x;

% figure(8)
% plot(x,y,'b',x,-y,'b')

F.3.1 Poly-Tie Shaped Structures

function width = PolyTieFunction(x, Wo, Wm, a, b, l, DeviceType, order, c, d, nx)
%------------------------------------------------------------------------
% Written by B.D. Davidson 2010
% Outputs an array containing the width of the structure corresponding to
% nodal locations of the FEM mesh
%
the shape is determined by fitting a given order polynomial to a a few
given points \( Wo, Wm, a, b, c, d \) etc. The number of points can be
increased as desired by the user
\( a \) and \( b \) are x coordinates and \( c \) and \( d \) are y coordinates for points
that help define the curvature of the shape near L/2

\[
\begin{align*}
\text{s} &= \text{warning('off', 'MATLAB:polyfit:PolyNotUnique');} \\
\text{if nargin} < 8  \\
&\quad \quad c = Wo + Wo*0.1; \\
&\quad \quad d = c; \\
\text{end} \\
\text{if DeviceType == 1}  \\
&\quad xr = [0 \ a \ 1/2 \ b \ l];  \\
&\quad yr = [Wm \ c \ Wo \ d \ Wm]; \\
\text{else}  \\
&\quad xr = [0 \ a \ l];  \\
&\quad yr = [Wm \ c \ Wo]; \\
\text{end} \\
\text{fit the points}  \\
[P] &= \text{polyfit(xr, yr, order);} \\
yd &= \text{zeros(length(x),1);} \\
\text{switch DeviceType}  \\
&\quad \text{case 1} \\
&\quad \quad flag = \text{find(x == 1/2);} \\
&\quad \quad y(1:flag,1) = \text{polyval(P,x(1:flag));} \quad \% \text{Y is the half width}
k = 0;
for i = 1:length(y)
    yus(i,1) = y(end-k);
k = k+1;
end

yd(1:length(y)) = y;
if length(x) > nx+1;
    yd(flag+1:end,1) = yus;
else
    yd(flag:end,1) = yus;
end
y = yd;
otherwise
    y = polyval(P,x);
end

width = 2*y;  % The total width

plot(xr, yr, '.', x, y, 'b', x,-y, 'b')  % plot the structure
grid on

F.4  Mesh Generators

F.4.1  Mesh Generator for Mechanical Domain

function [fecoord, fetopo, feprop, febc, numfenod, numfele]...
    = BeamMesherCoupled(s, l, h, nx, ny);
% Define the Super-Element

ndnod=4;
ndeim=1;

dc = [0 0; %Node 1
     1 0; %Node 2
     0 h; %Node 3
     1 h]; %Node 4, Variable with design variable

dc1=zeros(ndnod,2);

% Making the Topology, ie, what are the Super elements?

% topology of design elements
% type of element, list of node numbers in order
%
% type: 1 Lagrange element
% type: 2 Coons element
%
% for Coons-elements: last node needs to first node

tp = [2 1 2 4 3 1];

% intervalls nx.ny and
% for Lagrange elements:  4 - 4 node element
% 8 - 8 node element
% for Coons patches: edge types (4 entries)
% 1 - linear edge    (2 nodes)
iv=[nx ny 1 1 1 1];

%% element property flag and fetyp

dprop=ones(ndele,1);
fetyp=3*ones(ndele,1);

%% boundary code for elemental edges
% 1 = source load
% 2 = drain load
% 3 = clamped edge

bcedg=zeros(ndele,4);

% bcedg(2,:)=[1 0 0 0]; % distributed load
% bcedg(4,:)=[0 0 0 2]; % clamped edge

bcedg(1,:) = [2 3 0 3];
% bcedg(2,:) = [2 3 0 3];
% bcedg(3,:) = [1 3 0 0];

% boundary code for control nodes;
bcdnod=zeros(ndnod,1);

%% generating fe mesh

if nargin == 2
[fecoord, fetopo, feprop, febc, numfenod, numfele, d_fecoord]...
    = meshgen(dc, tp, iv, dprop, bcedg, bcnod, fetyp, ndnod, ndele, d_dc);
else
    [fecoord, fetopo, feprop, febc, numfenod, numfele]...
    = meshgen(dc, tp, iv, dprop, bcedg, bcnod, fetyp, ndnod, ndele);
end

%% plot mesh using calfem's eldraw2

ex=zeros(numfele,4);
ey=zeros(numfele,4);

for i=1:numfele
    for j=1:4
        ex(i,j)=fecoord(fetopo(i,j+1),1);
        ey(i,j)=fecoord(fetopo(i,j+1),2);
    end
end

% eldraw2(ex,ey,[ 2, 1, 0]); % used to plot the mesh

F.5 Utilities

F.5.1 Global Stiffness and Mass Matrix Assembly for the Mechanical Domain

function [K M fecoord, fetopo, feprop, febc, numfenod, numfele, edof, Ex, Ey, ep, D]...
    = AssembleKM(E, v, ro, thick, s, l, h, nx, ny)

%% ---------------------------------------------------------------------

% This program was written by Bradley Darren Davidson, and uses codes
% provided by the CalFEM package as well as Dr. Kurt Maute
%
% Written March 6 2009
%% This meshes the input geometry and outputs all relevant information
%% such as the element coordinates, number of elements, boundary flags,
%% number of nodes, and number of elements

[fecoord,fetopo,feprop,febc,numfenod,numfele]=BeamMesherCoupled(s,l,h,nx,ny);

%% Construct constitutive matrix

[D] = hooke(1,E,v); % CalFEM code

%% Construct elemental degrees of freedom

Dof=zeros(numfenod,2);

for i=1:numfenod
    Dof(i,1)=(i-1)*2+1;
    Dof(i,2)=(i-1)*2+2;
end

edof=zeros(numfele,9);
edof(:,1)=(1:1:numfele)';

for i=1:numfele
    for j=1:4
        edof(i,2+(j-1)*2)=Dof(fetopo(i,j+1),1);
        edof(i,3+(j-1)*2)=Dof(fetopo(i,j+1),2);
    end
end
[Ex,Ey]=coordxtr(edof,fecoord,Dof,4);  % Extracts the elemental coordinates

%% Construct Global Stiffness/ Mass Matrices

K = zeros(2*numfenod,2*numfenod);
f = zeros(2*numfenod,1);

for i = 1:numfele
    coord = fetopo(i,2:3)';
    coord = fecoord(coord,1);
    for j = 1:2
        found = find(abs((thick(:,1)-coord(j,1)))<1e-8);
        flgcoord(j,1) = found(1);
    end
    thk = mean([thick(flgcoord(2),2),thick(flgcoord(1),2)]);
    ep(i,:) = [1 thk 2];
end

for i = 1:numfele
    [Ke Fe] = plan4e(Ex(i,:),Ey(i,:),ep(i,:),D);  % CalFEM code
    [K f] = assem(edof(i,:),K,Ke,f);
end

M = zeros(2*numfenod,2*numfenod);
for i = 1:numfele
    [Me]=plani4m(Ex(i,:),Ey(i,:),ep(i,:),ro); % CalFEM code
    [M]=assem(edof(i,:),M,Me);
end

F.5.2 Faux Global Stiffness Assembly for the Electrostatic Domain

function [K fecoord,fetopo,feprop,febc,numfenod,numfele,edof,Ex,Ey,ep,D]...
    = Assemble_K_Efield(E,v,ro,thick,i,h,nx,ny,EleCase)
% This program was written by Bradley Darren Davidson, and uses codes
% provided by the CalFEM package as well as Dr. Kurt Maute
%
% Written March 6 2009
%------------------------------------------------------------------------------
%% Use mesher program to mesh beam
[fecoord,fetopo,feprop,febc,numfenod,numfele]=EfieldMesher(i,h,nx,ny);

% build constitutive matrix
[D] = hooke(1,E,v);

% construct elemental degrees of freedom
Dof=zeros(numfenod,2);

for i=1:numfenod
    Dof(i,1)=(i-1)*2+1;
    Dof(i,2)=(i-1)*2+2;
end

edof=zeros(numfele,9);
edof(:,1)=(1:1:numfele)';

for i=1:numfele
    for j=1:4
        edof(i,2+(j-1)*2)=Dof(fetopo(i,j+1),1);
        edof(i,3+(j-1)*2)=Dof(fetopo(i,j+1),2);
    end
end

[Ex,Ey]=coordxtr(edof,fecoord,Dof,4);

%% construct Stiffness/ Mass Matrices

ep = [1 thick 2];

m = 1;
n = 1;
for i=1:numfele
    if EleCase == 0
        [Kele]=plani4e(Ex(i,:),Ey(i,:),ep,D,[0;0]);
    else
        [fei,Kele]=plani4nl(Ex(i,:),Ey(i,:),ep,edof(i,2:9),D,[0;0]);
    end
    for j = 1:8
        for k=1:8
            if Kele(j,k) ≠ 0
                KBuilder(m,:) = [edof(i,j+1) edof(i,k+1) Kele(j,k)];
                m = m+1;
            end
        end
    end
end
K = sparse(KBuilder(:,1),KBuilder(:,2),KBuilder(:,3),2*numfenod,...
    2*numfenod,length(KBuilder));

**F.5.3 Elemental Capacitance for Three-Terminal Devices**

```matlab
function [Cap gl_el d_el gr_el] = Capacitance3t(U,nls,fecoord,extents,Wo,Wm,DeviceType,PC)
% Written By Bradley Darren Davidson 2010
% this function computes the elemental capacitance based on the
% discretation of a parallel plate capacitor model

eps = 8.85e-12;

a = 1:2*nls(end);
disp = U(a);
```
disp\mathbf{x} = \text{disp}(1:2:\textbf{end}); disp\mathbf{y} = \text{disp}(2:2:\textbf{end});

%graduate the source nodes
\begin{align*}
&[\text{newcoord gridx gridy spacing nelements gradcoord}]... \\
&= \text{gradiatednodes}(\text{extents, fecoord,nls});
\end{align*}

\begin{align*}
&[\text{dispx\_coord gridx gridy spacing nelements gradcoord}]... \\
&= \text{gradiatednodes}(\text{extents, fecoord,nls,dispx});
\end{align*}

\text{dispx} = \text{dispx\_coord}(:,2);

\begin{align*}
&[\text{dispy\_coord gridx gridy spacing nelements gradcoord}]... \\
&= \text{gradiatednodes}(\text{extents, fecoord,nls,dispy});
\end{align*}

\text{dispy} = \text{dispy\_coord}(:,2);

\begin{align*}
\text{for } i = 1:\text{length(dispy)} \\
\quad \text{disp}(2*i-1:2*i,1) &= \left[\text{dispx}(i);\text{dispy}(i)\right];
\end{align*}

\text{Uc} = \text{CenterDisplacements}(\text{disp},1:1:\text{length(dispy)});

%%% need new areas

\begin{align*}
\text{if } \text{PC} &= 0 \\
\quad \text{Wm} &= \text{Wo};
\end{align*}

\begin{align*}
\quad \text{widths} &= \text{BowTieFunction(gridx, Wo, Wm, extents(1), extents(2),...} \\
\quad &\text{gridx(end), DeviceType});
\end{align*}

\begin{align*}
\text{elseif } \text{PC} &= 1
\end{align*}

\begin{align*}
\text{order} &= 9; \% \text{order polynomial for fit}
\end{align*}
widths = PolyTieFunction,2T(gridx,Wo,Wm,extents(1),...
    extents(2),gridx(end),DeviceType,order,.3,.3,length(dispy));

elseif PC == 2

widths = BowTieFunction( gridx,Wo,Wm,extents(1),...
    extents(2),gridx(end),DeviceType);
end

thick(:,1) = gridx; thick(:,2) = widths; % first column is coordinates,
% 2nd column is widths

for i = 1:length(thick)-1;
    meanthick(i,1) = mean([thick(i+1,2),thick(i,2)]);
end

for i = 1:length(gridx)-1
    lel(i,1) = gridx(i+1,1)-gridx(i);
end
Area = lel.*meanthick;

%%% Capacitances

gatel = find(gridx <= extents(1));
gater = find(gridx >= extents(2));
drain = (gatel(end)+1:1:gater)';

a = length(gatel)-1;
b = length(gater)-1;
c = length(drain)-1;
gl_el = 1:1:a;
d_el = (a+1):1:(a+c);
gr_el = a+c+1:1:a+b+c;

gapd = extents(end)-extents(end-1);
gapg = extents(end);

Cap(gl_el) = eps.*Area(gl_el)./(gapg+Uc(gl_el));
Cap(d_el) = eps.*Area(d_el)./(gapd+Uc(d_el));
Cap(gr_el) = eps.*Area(gr_el)./(gapg+Uc(gr_el));

**F.5.4** Displacement of Element Centers

```matlab
function Uc = CenterDisplacements(U,nls)
%------------------------------------------------------------------------
% Written By Bradley Davidson
% % Calculates the center displacement of an element as the mean of the % nodal displacements
% %------------------------------------------------------------------------
% h = length(nls);
Uc = zeros(h-1,1);
for k = 1:h-1
    Uc(k,1) = (U(2*nls(k+1),1)+U(2*nls(k),1))/2;
end
```

**F.5.5** Nodal Charge for Three-Terminal Devices
function [Qnodal] = Charge3t(Cap,Voltagedrain,Voltagegate,...
VDD,coord,extents,nls,t,SubCase,gl_el,d_el,gr_el)

% Written By Bradley Darren Davidson 2010

% this function computes the nodeal charge for calculation of the
% electrostatic forces acting on the beam

% close all;clear all;clc
% load test4charge.mat
% t = t(3);
% coord = fecoord;
% Voltagegate = Vg;
% Voltagedrain = Voltage;
%************%

% need to find the coordinates of the drain

[coord gridx gridy spacing nelements gradcoord]...
    = gradiatednodes(extents, coord,nls);  %gradiate the source nodes

switch SubCase
    case 1
        Q(gl_el) = (Voltagegate-VDD)*Cap(gl_el);
        Q(gr_el) = (Voltagegate-VDD)*Cap(gr_el);
        Q(d_el) = (Voltagedrain*t-VDD)*Cap(d_el);
case 2
    Q(gl_el) = (Voltagegate*t-VDD)*Cap(gl_el);
    Q(gr_el) = (Voltagegate*t-VDD)*Cap(gr_el);
    Q(d_el) = (Voltagedrain-VDD)*Cap(d_el);
otherwise
    Q(gl_el) = (Voltagegate*t-VDD)*Cap(gl_el);
    Q(gr_el) = (Voltagegate*t-VDD)*Cap(gr_el);
    Q(d_el) = (Voltagedrain*t-VDD)*Cap(d_el);
end

del = gridx(2,1) - gridx(1,1);
k = 1;
j = 0;

for i = 1:nls(end)  % find the nodal numbers...
    f(i,1) = find(abs((gridx - (i-1)*del))<1e-3);
    k = k+1;
end

%% nodal charge
    Qnodal = zeros(1,length(Q)+1);
    j = 1;
    for i = 1:length(Q)
        dum(j,i:i+1) = [Q(i)/2 Q(i)/2];
        j = j+1;
    end

    for i = 1:j-1
        Qnodal = Qnodal+dum(i,:);
    end
    Qnodal = Qnodal(f);
function febc = DrainBcs(fecoord, febc, extents, elx, ely, nxref, nyref);

%------------------------------------------------------------------------
% Written By Bradley Davidson
% %
% % Calculates the boundary condition flag for the drain electrode
% %------------------------------------------------------------------------

flx = find(fecoord(1:nxref+1,1)<extents(1));
f2x= find(fecoord(1:nxref+1,1)>extents(2));

min_x = fecoord(flx(end),1);
max_x = fecoord(f2x(1),1);

range_x = (min_x:elx:max_x)';
range_y = (0:ely:extents(4))';

k = 1;
for j = 1:length(range_y)
    for i = 1:length(range_x)
        dc(k,:) = [range_x(i) range_y(j)];
        k = k+1;
    end
end
k =1;
for j = 1:length(dc)
    for i = 1:length(fecoord)
dum(i,:) = fecoord(i,:) - dc(j,:);

end
flagged = find(abs(sum(dum'))<1e-4);
fbc(k,1) = flagged(1);

k = k+1;
end

febc(fbc,1) = 3;

**F.5.7 Electrostatic Domain Refinement to include Drain Geometry and Coordinates**

```matlab
function [coord gridx gridy spacing nelements gradcoord WD cmidx]...
    = DrainFieldCoords(extents, coord, elx, ely, h,nxref,nyref,u)
%
% Written By Bradley Darren Davidson 2010
%
% This function calculates new coordinate points to add to the mesh which
% represent the inclusion of a drain into the electrostatic domain
%
%*******************************************************************************
%
%*******************************************************************************

% close all;clear all;clc
% load test4drain.mat   %for testing
%*******************************************************************************
flagu = 2:2:length(u);
delu_y = mean(u(flagu));
ll = nxref+1;
for B = 1:nyref+1;

    \%\% find coordinates at the left bound

    flagl = find(coord((B-1)*ll+1:B*ll,1) \leq extents(1))+(B-1)*ll;
    clx = coord(flagl(end),1);

    if flagl(1) \neq 1;
        check = abs(coord(flagl(1)-1,1)-extents(1));
        if check <1e-6
            clx = coord(flagl(1)-1,1);
        end
    end

    \%\% find coordinates at the right bound

    flagr = find(coord((B-1)*ll+1:B*ll,1) \geq extents(2))+(B-1)*ll;
    crx = coord(flagr(1),1);

    \% strange error check

    if flagr(1) \neq 1;
        check = abs(coord(flagr(1)-1,1)-extents(2));
        if abs(coord(flagr(1)-1,1)-extents(2)) <1e-6 \&\& flagr(1) \neq 1
            crx = coord(flagr(1)-1,1);
        end
    end

    num = round((crx -clx)/elx);

    cmidx = [];

for i = 1:num-1
    cmidx(i) = clx+i*elx;
end

if abs(clx-extents(1))>1e-3 || abs(crx-extents(2))> 1e-3

% adding the new xcoords for the gradiated drain region

dspacel = (extents(1)-clx)/(4);
coord2l = clx:dspacel:extents(1);

if length(cmidx) == 1
    dspace = (extents(2)-extents(1))/(8*5);
    coord2c = extents(1):dspace:extents(2);
    WD = 0;
else
    coord2c = [extents(1) cmidx extents(2)];
    dspace = (extents(2)-extents(1))/length(coord2c);
    WD = 1;
end

dspacer = (crx-extents(2))/(4);
coord2r = extents(2):dspacer:crx;

a = length(coord2l); b = length(coord2c); c = length(coord2r);

coordx = zeros(a+b+c-2,1);
coordx(1:a,1) = coord2l';
coordx(a:a+b-1,1) = coord2c';
coordx(a+b-1:end,1) = coord2r';
%% some outputs that will remain unchanged from here on out...

telements(B,1) = (a+b+c-3)-num;

gradcoord(B,:) = [clx cmidx crx];

spacing(B,:) = [dspacel dspace dspacer];

%% need to calculate the y coordinates for the gradiated drain region
cly = coord(flagl(end),2);
cry = coord(flagr(1),2);

flagmid = find(abs((coord((B-1)*ll+1:B*ll,1)...
   -cmidx((length(cmidx)-1)/2+1))+delu_y)/cmidx(end)<1e-2)...
   +(B-1)*ll; % this will change with every loop

cmpidy = coord(flagmid,2);

P = polyfit([clx cmidx((length(cmidx)-1)/2+1) crx],...
   [cly cmidy cry],2);

coordy = polyval(P,coordx);

% plot(coordx, coordy,'b',[clx cmidx crx], [cly cmidy cry],'r')

%% organize the coordinates properly

xcoords = coord((B-1)*ll+1:B*ll,1);
ycoords = coord((B-1)*ll+1:B*ll,2);
a = length(xcoords);
b = length(coordx)-2;
dumx = zeros(a+b,1);
dumy = dumx;
dumx(1:a,1) = xcoords;
dumy(1:a,1) = ycoords;
dumx(a+1:end,1) = coordx(2:end-1,1);  % unsorted xcoords
dumy(a+1:end,1) = coordy(2:end-1,1);

xcoords = sort(dumx);  % sorted xcoords
ycoords = zeros(size(xcoords));

for i = 1:length(xcoords)
    flagsort = find(abs(xcoords-dumx(i))<1e-5);
    ycoords(flagsort(1),1) = dumy(i);
end

% need to remove multiples from the coordinates
a = length(xcoords);
k = 1;
for i = 1:a-1
    if abs(xcoords(i)-xcoords(i+1))<1e-5
        flag(k,1) = i+1;
        k = k+1;
    end
end

xcoords(flag) = [];  % sorted xcoords with multiples removed
ycoords(flag) = [];

a = length(xcoords);

coord_update((B-1)*a+1:B*a,:) = [xcoords ycoords];

else
spacing(B,:) = [elx elx elx];
elements(B,1) = 0;
gradopt(B,:) = [clx cmidx((length(cmidx)-1)/2+1) crx];
WD = 0;
coord_update = coord;
xcoords = coord(1:nxref+1,1);
coody = (0:ely:extents(5))';

end
end

%% outputs
coord = coord_update;

gridx = xcoords;
gridy = coody;

F.5.8 Drain Coordinate Transformation to Row and Column Space

function [draingrid dglbc dgrbc dgtbc dginterior]...
    = Drainmeshlocations_3t(nx, ny, draincoord, draincoordl,...
        draincoordr, draincoordt, spacing,elx, ely,gradcoord)

%-----------------------------------------------}
% Written By Bradley Darren Davidson 2010
%
% This Function takes the coordinates in cartesian space and transforms
% them to row column space, in this way we may avoid coordinates and speak
% about a nodes location as in it's row and column number in the finite
% difference mesh representation
%
%-----------------------------------------------}
% close all; clear all; clc
% load test4loc.mat
%
% nx = nelements + nxref;
% ny = nyref;

% full grid
mindx = min(draincoord(:,1));
maxdx = max(draincoord(:,1));

nx = round(mean(nx));

r = ny+1; % number of rows
c = nx+1; % number of columns

% range 1
els1 = gradcoord(1)/elx;

% range 2
els2 = (mindx - gradcoord(1))/spacing(1);

% range 3
els3 = (gradcoord(3) - maxdx)/spacing(3);

% grid points of the drains
dumfull = zeros(size(draincoord));
dumfull(:,1) = r - draincoord(:,2)/ely;

for i = 1:length(dumfull)
    dumfull(i,2) = els1+els2+1+ (draincoord(i,1)-mindx)/spacing(1,2);
end

draingrid = round(dumfull);

%% left side

duml = draincoordl;
duml(:,1) = r - draincoordl(:,2)/ely;
% duml(:,2) = c - draincoordl(:,1)/elx;

for i = 1:length(duml)
    duml(i,2) = els1+els2+1+ (draincoordl(i,1)-mindx)/spacing(1,2);
end

dglbc = round(duml);

%% right side

dumr = draincoordinr;
dumr(:,1) = r - draincoordinr(:,2)/ely;
% dumr(:,2) = c - draincoordinr(:,1)/elx;

for i = 1:length(dumr)
    dumr(i,2) = els1+els2+1+ (draincoordinr(i,1)-mindx)/spacing(1,2);
end
dgrbc = round(dumr);

%% top side
dumt = draincoordt;

dumt(:,1) = r - draincoordt(:,2)/ely;
% dumt(:,2) = c - draincoordt(:,1)/elx;

% for i = 1:length(dumt)
    dumt(:,2) = els1+els2+1+(draincoordt(:,1)-mindx)/spacing(1,2);
% end

dgtbc = round(dumt);

dglbc = sort(dglbc);
dgrbc = sort(dgrbc);
dgtbc = sort(dgtbc);

%% interior grid points

dginterior = draingrid;
k = 1;
for i = 1:length(dglbc)
    for j = 1:length(draingrid)
        if sum(dglbc(i,:) == draingrid(j,:)) == 2
            flagin(k,1) = j;
            k = k+1;
        end
    end
end
for i = 1:length(dgrbc)
    for j = 1:length(draingrid)
        if sum(dgrbc(i,:) == draingrid(j,:)) == 2
            flagin(k,1) = j;
            k = k+1;
        end
    end
end

for i = 1:length(dgtbc)
    for j = 1:length(draingrid)
        if sum(dgtbc(i,:) == draingrid(j,:)) == 2
            flagin(k,1) = j;
            k = k+1;
        end
    end
end

dginterior(sort(flagin),:) = [];

F.5.9 Drain Coordinate Finder/Flagger

function [draincoord,draincoordl, draincoordr, draincoordt]...
    = DrainSorter_3T(coord,nx,ny,drainextents,u,WD,cmidx)

%--------------------------------------------------------------->>
% Written By Bradley Darren Davidson 2010
%
% This function locates coordinate points of the drain in the array of all
% coordinates. We will require these points to solve laplaces equation for
% the domain.
%
%-----------------------------------------------------------------------

% % %**************************
% close all;clear all;clc
% load test4sorter.mat
% nx = spacing(2,2);
% ny = ely;
%
% %**************************

flagu = 2:2:length(u);
delu_y = mean(u(flagu));

err = 1e-3;
r = 1;

if WD == 0
drx = drainextents(1):nx:drainextents(2);
else
drx = [drainextents(1) cmidx drainextents(2)];
end

dry = drainextents(3):ny:drainextents(4);

for j = 1:length(dry)
    for i = 1:length(drx)
for k = 1:length(coord)
    if abs(coord(k,:) - [drx(i) dry(j)+delu_y])<[err err];
        flagdrain(r,1) = k;
        r = r+1;
    end
end

end

for i = 1:length(flagdrain)
    draincoord(i,:) = coord(flagdrain(i),:);
end

%%% drain boundaries

% left boundary

flagl = find(abs(draincoord(:,1) - drainextents(1))< err);


% right boundary

flagr = find(abs(draincoord(:,1)-drainextents(2))< err);

% top boundary

flagt = find(abs(draincoord(:,2)-(drainextents(4)+delu_y))< err);

fmax = max(draincoordt(:,2));
fmin = min(draincoordt(:,2));

if abs((fmax-fmin))>err
    check = round(ny/(fmax-fmin));
else
    check = 0;
end

if check == 1
    draincoordt(1:length(drx),:) = [];
end

%% plotting for visualization

%% for i = 1:length(coord)
%%     plot(coord(i,1),coord(i,2),'.b')
%%     hold on
%% end

%% for i = 1:length(draincoord)
%%     plot(draincoord(i,1),draincoord(i,2),'r')
%%     hold on
%% end

%% for i = 1:length(draincoordl)
%%     plot(draincoordl(i,1),draincoordl(i,2),'g')
%%     hold on
%% end

%% for i = 1:length(draincoordr)
%%     plot(draincoordr(i,1),draincoordr(i,2),'g')
%%     hold on
for i = 1:length(draincoordt)
    plot(draincoordt(i,1),draincoordt(i,2),'.g')
end

F.5.10 Coordinates of the Deformed Electrostatic Domain

function [coord] = ElectricFieldCoords_v2(coord,disp)
% function [coord gps] = ElectricFieldCoords(xmin,xmax,ymin,ymax,nx,ny,disp)

flagx = (1:2:length(disp))';
flagy = (2:2:length(disp))';
coord(:,1) =coord(:,1)+disp(flagx);
coord(:,2) = coord(:,2)+disp(flagy);

F.5.11 Electrostatic Force

function [fe] = ElectroStaticForce(Qnodal, Efx, Efy, flagu, numfenod)

% Written By Bradley Darren Davidson 2010
% This program will calculate the electrostatic force
% based on the Efield and calculated charge
%-----------------------------------------------------------------------

%%% Need to distribute the charge, a scalar value, to the elemental nodes

fey = Qnodal.*Ef_y;
fex = Qnodal.*Ef_x;

fe = sparse(2*numfenod,1);
for i = 1:length(flagu)/2
    fe(flagu(2*i-1),1) = fex(i);
    fe(flagu(2*i),1) = fey(i);
end

fe = fe*1e6; % scaling parameter due to choice of units

F.5.12 Mesh Refinement

function [coord gridx gridy spacing nelements gradcoord]...
    = gradiatednodes(extents,coord,nls,Y)

%**************************
% close all;clear all;clc
% load test4charge.mat
% coord = fecoord;
%**************************

if nargin >3
    coord(1:nls(end),2) = Y;
end

end
elx = coord(2,1)-coord(1,1);
ely = elx;
ll = nls(end);
for B = 1:1;

%% find coordinates at the left bound
flagl = find(coord((B-1)*ll+1:B*ll,1)<extents(1))+(B-1)*ll;
clx = coord(flagl(end),1);

%% find coordinates at the right bound
flagr = find(coord((B-1)*ll+1:B*ll,1)>extents(2))+(B-1)*ll;
crx = coord(flagr(1),1);

%% find coordinates at the mid nodes;
um = round((crx-clx)/elx);

for i = 1:num-1
    cmidx = clx+i*elx;
end

%% adding the new xcoords for the gradiated drain region
dspacel = (extents(1)-clx)/4;
coord2l = clx:dspacel:extents(1);

dspace = (extents(2)-extents(1))/8;
coord2c = extents(1):dspace:extents(2);

dspacer = (crx-extents(2))/4;
coord2r = extents(2):dspace:crx;

a = length(coord2l); b = length(coord2c); c = length(coord2r);
coordx = zeros(a+b+c-2,1);
coordx(1:a,1) = coord2l';
coordx(a:a+b-1,1) = coord2c';
coordx(a+b-1:end,1) = coord2r';

%% some outputs that will remain unchanged from here on out...

nelements(B,1) = (a+b+c-3)-num;

gradcoord(B,:) = [clx cmidx crx];

spacing(B,:) = [dspacel dspace dspacer];

%% need to calculate the y coordinates for the gradiated drain region
% if nargin > 3

cly = coord(flagl(end),2);
cry = coord(flagr(1),2);

flagmid = find(abs((coord((B-1)*ll+1:B*ll,1)-cmidx)/cmidx)<1e-4)+(B-1)*ll;
cmidy = coord(flagmid,2);

P = polyfit([clx cmidx crx], [cly cmidy cry],2);
coordy = polyval(P,coordx);

% end

%% organize the coordinates properly

xcoords = coord((B-1)*ll+1:B*ll,1);
ycoords = coord((B-1)*ll+1:B*ll,2);
a = length(xcoords);
b = length(coordx)-2;
dumx = zeros(a+b,1);
dumy = dumx;
dumx(1:a,1) = xcoords;
dumy(1:a,1) = ycoords;
dumx(a+1:end,1) = coordx(2:end-1,1); %unsorted xcoords
dumy(a+1:end,1) = coordy(2:end-1,1);

xcoords = sort(dumx); %sorted xcoords
ycoords = zeros(size(xcoords));

for i = 1:length(xcoords)
    flagsort = find(abs(xcoords-dumx(i))<1e-3);
    ycoords(i,1) = dumy(flagsort(1));
end

% need to remove multiples from the coordinates
a = length(xcoords);
k = 1;
for i = 1:a-1
    if abs(xcoords(i)-xcoords(i+1))<1e-3
        flag(k,1) = i;
        k = k+1;
    end
end

xcoords(flag) = [];
ycoords(flag) = [];
a = length(xcoords);

coord_update((B-1)*a+1:B*a,:) = [xcoords ycoords];
%% put it all back together
% k = 1;
% for j = 1:length(coordy)
%     for i = 1:a
%         coord(k,:) = [xcoords(i) coordy(j)];
%         k = k+1;
%     end
% end
end

%% outputs
coord = coord_update;

gridx = xcoords;
gridy = coordy;

F.5.13 Gradient of the Potential for a Three-Terminal Device

function [fx fy] = Gradient_3T(potential,rx,ry,coord,dglbc,dgrbc,dgtbc,nx,ny)

%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% This program will compute the potential between deformed plates for
% my NEMS devices
% Outputs: gradient of the potential at each point in the electrostatic
% domain
%-----------------------------------------------------------------------

%% top
fx = zeros(ny+1,nx+1);
fy = fx;
nx = round(mean(nx));

for i = 1
for j = 2:nx
    fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
    fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));
end
end

% corners

j = 1;

fx(i,j) = (potential(i,j+1)-potential(i,j))/(rx(i,j));
fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));

j = nx+1;

fx(i,j) = (potential(i,j)-potential(i,j-1))/(rx(i,j));
fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));

%% bottom Surfaces

% left gate BOTTOM section

for i = ny+1 %last row
    for j = 2:dglbc(1,2)-1 % interior columns
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));
    end
end
end
end

% left gate corners

j = 1;

% fx(i,j) = (potential(i,j+1)-potential(i,j))/(rx(i,j));
yi(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));

j = dglbc(1,2);

% fx(i,j) = (potential(i,j)-potential(i,j-1))/(rx(i,j));
yi(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));

% right gate BOTTOM section

for i = ny+1  %last row
    for j = dgrbc(1,2)+1:nx  % interior columns
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
yf(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));
    end
end

% right gate corners

j = dgrbc(1,2);

fy(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));

j = nx+1;
\[ f_y(i,j) = \frac{\text{potential}(i,j) - \text{potential}(i-1,j)}{r_y(i,j)}; \]

% drain BOTTOM section

for \( i = \text{dgtbc}(1,1) \) %last row
    for \( j = \text{dglbc}(1,2)+1: \text{dgrbc}(1,2)-1 \) % interior columns
        \[ f_x(i,j) = \frac{\text{potential}(i,j+1) - \text{potential}(i,j-1)}{2*r_x(i,j)}; \]
        \[ f_y(i,j) = \frac{\text{potential}(i,j) - \text{potential}(i-1,j)}{r_y(i,j)}; \]
    end
end

%% sides with Dirchlet bc

% this loop takes care of the left and right sides where there is no Ex field

for \( i = 2: \text{ny} \) %interior for rows
    for \( j = [1 \ \text{nx}+1] \) % first and last column
        \[ f_y(i,j) = \frac{\text{potential}(i+1,j) - \text{potential}(i-1,j)}{2*r_y(i,j)}; \]
    end
end

% this loop will take care of the electrically isolated area between the drain and gate electrodes

for \( i = \text{dgtbc}(1,1)+2: \text{ny} \) %interior for rows
    for \( j = [\text{dglbc}(1,2) \ \text{dgrbc}(1,2)] \) % first and last column
        \[ f_y(i,j) = \frac{\text{potential}(i+1,j) - \text{potential}(i-1,j)}{2*r_y(i,j)}; \]
    end
end
%% Interior

for i = 2:dgtbc(1,1)
    for j = 2:nx
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i+1,j)-potential(i-1,j))/(2*ry(i,j));
    end
end

for i = dgtbc(1,1):ny
    for j = 2:dglbc(1,2)-1
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i+1,j)-potential(i-1,j))/(2*ry(i,j));
    end
end

for i = dgtbc(1,1):ny
    for j = dgrbc(1,2)+1:nx
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i+1,j)-potential(i-1,j))/(2*ry(i,j));
    end
end

F.5.14 Pull-in Voltage

function pi = Pullin_MP(U,t,Voltage, Vg, AnalysisType,...
    ActuationType,extents,InvContact)

%---------------------------------------------------------------

% Written By Bradley Darren Davidson 2010
%Extracts pull-in voltage from displacement data

switch AnalysisType
    case 10
        k = 1;
        for i = 1:length(U)
            if U(i)<-extents(5)*.4
                flag(k) = i;
                k = k+1;
            end
        end
    end

if k ==1
    flag = 0;
end

if sum(flag) == 0
    pi = t(end)*Voltage;
else
    pi = t(flag(1))*Voltage;
end
otherwise

switch ActuationType
    case 1
        k = 1;
        for i = 1:length(U)
            if U(i)<-(extents(5)-extents(4))*4
                flag(k) = i;
            end
        end
\begin{verbatim}
    k = k+1;
    end
end

if k == 1
    flag = 0;
end

if sum(flag) == 0
    pi = t(end)*Voltage;
else
    pi = t(flag(1))*Voltage;
end

\textbf{case} \{2,0\}
    k = 1;
    for i = 1:length(U)
        if U(i)<-extents(5)*.4
            flag(k) = i;
            k = k+1;
        end
    end
end

if k == 1
    flag = 0;
end

if sum(flag) == 0
    pi = t(end)*Vg;
else
    pi = t(flag(1))*Vg;
\end{verbatim}
otherwise

if ActuationType == 2 && InvContact == 1
    k = 1;
    for i = 1:length(U)
        if U(i) < -(extents(5) - extents(4))
            flag(k) = i;
            k = k + 1;
        end
    end
end

if k == 1
    flag = 0;
end

if sum(flag) == 0
    pi = t(end) * Vg;
else
    pi = t(flag(1)) * Vg;
end
end
end

F.5.15 Residual

function [R Kt fi ek in epot] = Res(Un, Vn, An, fext, fdof, Ex, ... 
    Ey, numfele, numfenod, edof, ep, D, ro, tstep, beta, Case, Kelectric)

% ------------------------------------------>>
Kt = zeros(2*numfenod,2*numfenod);
Mt = zeros(2*numfenod,2*numfenod);
fi = zeros(2*numfenod,1);

ekin = 0;
epot = 0;

for k = 1:numfele
  ed = extract(edof(k,:),Un);
edd = extract(edof(k,:),Vn);
[Ke] = plani4e(Ex(k,:),Ey(k,:),ep,D);
fe = Ke*ed';

[Me]=plani4m(Ex(k,:),Ey(k,:),ep,ro);
[Kt fi]=assem(edof(k,:),Kt,Ke,fi,fe);
[Mt]=assem(edof(k,:),Mt,Me);

  ekin = ekin + 0.5*edd*Me*edd';
  epot = epot + 0.5*ed*Ke*ed';
end

Mt = sparse(Mt);
Kt = sparse(Kt);

switch Case
  case {6,7,8,9}
\[ f_{ii} = K_{electric} \times U_{n}; \]
\[ R = M_{t} \times A_{n} + f_{i} - f_{ext} - f_{ii}; \]
\[ K_{t} = \frac{1}{(\beta \times t_{step}^2)} \times M_{t} + K_{t} - K_{electric}; \]

\textbf{otherwise}\]
\[ R = M_{t} \times A_{n} + f_{i} - f_{ext}; \]
\[ K_{t} = \frac{1}{(\beta \times t_{step}^2)} \times M_{t} + K_{t}; \]
\textbf{end}\n
\textbf{F.5.16 Plotter}\n
\textbf{function} \ y = \text{PoincarePlots}\_\text{MP}\(U, V, A, t, \text{forcehistory}, \text{ekinhistory},...\)
\(\text{epothistory}, \text{events}, \text{Voltage}, \text{Voltage}_{\text{gate1}},...\)
\(\text{Voltage}_{\text{gate2}}, \text{VAC,A}\text{na}\text{lysisType,A}\text{cuationType})\n
\%-----------------------------------------------------------------------
\% Written By Bradley Darren Davidson 2010
\% % Outputs every plot of interest
\% % %-----------------------------------------------------------------------

\text{mkr =6;}
\text{NLC = ' linear Elements';}

\text{figure(3)}
\text{subplot(2,2,1)}
\text{plot(U,V,'.','markersize',mkr)}
\text{title(['Displacement-Velocity Phase Plane: V.D.R.A.I.N = '...\n\text{num2str(Voltage) ' VAC = ' num2str(VAC) NLC ' V.G.A.T.E.1 = '...\n\text{num2str(Voltage\text{gate1}) 'V.G.A.T.E.2 = ' num2str(Voltage\text{gate2})})]}
xlabel('Displacement [um]')
ylabel('Velocity [um/s]')
grid on

% figure(4)
subplot(2,2,2)
plot(U,A,'.','markersize',mkr)
title(['Displacement-Acceleration Phase Plane: V_D_R_A_I_N = '...
       num2str(Voltage) ' VAC = ' num2str(VAC) NLC ' V_G_A_T_E_1 = '...
       num2str(Voltage_gate1) 'V_G_A_T_E_2 = ' num2str(Voltage_gate2)])

xlabel('Displacement [um]')
ylabel('Acceleration [um/s^2]')
grid on

% figure(5)
subplot(2,2,3)
plot(V,A,'.','markersize',mkr)
title(['Velocity-Acceleration Phase Plane: V_D_R_A_I_N = '...
       num2str(Voltage) ' VAC = ' num2str(VAC) NLC ' V_G_A_T_E_1 = '...
       num2str(Voltage_gate1) 'V_G_A_T_E_2 = ' num2str(Voltage_gate2)])

xlabel('Velocity [um/s]')
ylabel('Acceleration [um/s^2]')
grid on

% figure(6)
subplot(2,2,4)
plot3(U,V,A,'.','markersize',mkr)
title(['Phase Space: V_D_R_A_I_N = ' num2str(Voltage) ' VAC = '...
       num2str(VAC) NLC ' V_G_A_T_E_1 = ' num2str(Voltage_gate1)...
       'V_G_A_T_E_2 = ' num2str(Voltage_gate2)])
xlabel('Displacement [um]')
ylabel('Velocity [um]')
zlabel('Acceleration [um/s^2]')
grid on

figure(4)
% figure(7)
subplot(2,1,1)
if ActuationType == 2
    plot(t(1:length(U))*Voltage_gate1,U(1:end))
xlabel('Gate Voltage [V]')
else
    plot(t(1:length(U))*Voltage,U(1:end))
xlabel('Voltage [V]')
end
% axis([0 t(length(U)) -gap .01])
title(['displacement V. Voltage: V_D_R_A_I_N = ' num2str(Voltage)...
     ' VAC = ' num2str(VAC) NLC ' V_G_A_T_E_1 = ' num2str(Voltage_gate1)...
     ' V_G_A_T_E_2 = ' num2str(Voltage_gate2)])
ylabel('Displacement [um]')
grid on

% % figure(8)
subplot(2,1,2)
if ActuationType == 1
    plot(t(1:length(U))*Voltage,V(1:end))
xlabel('Drain Voltage [Volts]')
else
    plot(t(1:length(U))*Voltage_gate1,V(1:end))
xlabel('Gate Voltage [Volts]')
end
axis([0 t(length(U)) min(V) max(V)])

title(['Velocity V. Time: VDC = ' num2str(Voltage) ' VAC = '...
num2str(VAC) NLC ' V.G.A.T.E.1 = ' num2str(Voltage_gate1)...
' V.G.A.T.E.2 = ' num2str(Voltage_gate2)])

% xlabel('time [s]')
ylabel('Velocity [um/s]')
grid on

% % figure(9)
figure(5)
subplot(2,2,1)
plot(t(1:length(U)),forcehistory)
title('forcehistory')
xlabel('time')
ylabel('force')
grid on

subplot(2,2,2)
plot(t(1:length(U)),sign(events(:,1)))
ylim([-2 2])
title('Event History')
xlabel('time')
ylabel('Eigen Frequency of Kt')
grid on

subplot(2,2,3)
plot(t(1:length(U)),ekinhistory)
F.5.17  Load Interpolation from Electric to Mechanical Domain

function [efy efx] = LoadDistribution3T(l,nx,gridx,Efy,Efx)

%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% %
% % This function maps the nodal E-field values calculated in the
% % Faux-Lagrangian domain to the mechanical domain via linear interpolation
% % of the values between the graduated mesh coordinates
% %
% %-----------------------------------------------------------------------

nodes = nx+1;    % Total Number of nodes in the mechanical domain
xmech = (0:1/nx:1)';  % x-coordinates of mech/elect surface
efy = zeros(1,nodes); % allocate some memory
efx = efy;

efy_me = Efy(1,:); % E-Field values calculated in the FL electric
efx_me = Efx(1,:); % domain, will be interpolated

for i = 2:length(gridx);
    nodel = 1:1:nodes;
    min = gridx(i-1); max = gridx(i);
    
    fmin = find(xmech < min);
    fmax = find(xmech ≥ max);
    [a b] = size(fmin);
    [c d] = size(fmax);
    
    if a == 0;
        nullify = fmax;
    else
        nullify = zeros(a+c,1);
        nullify(1:a,1) = fmin;
        nullify(a+1:end,1) = fmax;
    end
    nodel(nullify) = [];
    if sum(nodel)>1
        py = polyfit([gridx(i-1);gridx(i)],[efy_me(i-1);efy_me(i)],1);
        px = polyfit([gridx(i-1);gridx(i)],[efx_me(i-1);efx_me(i)],1);
        efy_aprox = polyval(py,xmech(nodel));
        efx_aprox = polyval(px,xmech(nodel));
    end
end
efx(nodel) = efx_aprox;
efy(nodel) = efy_aprox;
end

clear fmin fmax
end

F.6 Utilities Specific to 2-Terminal Simulations

F.6.1 Elemental Capacitance for 2-Terminal Devices

function [Cap] = Capacitance2t(Area, U, nls, gap)
% Written By Bradley Darren Davidson 2010
% this function computes the elemental capacitance based on the
% discretation of a parallel plate capacitor model
%------------------------------------------------------------------------

eps = 8.85e-12;
for j = 1:length(nls)-1
    Cap(1,j) = eps.*Area(j)./(gap+U(j,1)); % elemental Capacitance
end

F.6.2 Nodal Charge for 2-Terminal Devices

function [Qnodal] = Charge2t(Cap, Voltage, t)
% Written By Bradley Darren Davidson 2010
% this function computes the nodal charge: q = CV
%------------------------------------------------------------------------

Q = Voltage*t*Cap;
%%% nodal charge
Qnodal = zeros(1,length(Q)+1);
j = 1;
for i = 1:length(Q)
    dum(j,i:i+1) = [Q(i)/2 Q(i)/2];
j = j+1;
end
for i = 1:j-1
    Qnodal = Qnodal+dum(i,);
end

F.6.3 Coordinates of Deformed Electrostatic Domain Field Points for a 2-Terminal Device

function [coord gps]...
    = ElectricFieldCoords(coord,disp,xmin,xmax,ymin,ymax,nx,ny)

%-----------------------------------------------------------------------
% Written by Bradley Davidson 2010
% inputs: xmin, xmax, ymin, ymax describe region of interest
% nx and ny are the mesh refinements displacement is the displacement vector
% for the deformed beam's nodal points Outputs: coord is a matrix with the
% grid points
%-----------------------------------------------------------------------

  delx = (xmax-xmin)/nx;  dely = (ymax-ymin)/ny;
gps = [(xmin:delx:xmax)' (ymin:dely:ymax)'];

  flag = 1:2:length(disp);
  coord(1:length(disp)/2,1) = coord(1:length(disp)/2,1)+disp(flag,1);
  flag = 2:2:length(disp);
  coord(1:length(disp)/2,2) = coord(1:length(disp)/2,2)+disp(flag,1);
function [fx fy] = Gradient2t(potential,rx,ry,coord,nx,ny)
%%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% Outputs: gradient of the potential at each point in the electrostatic
% domain
%%-----------------------------------------------------------------------
%% top
for i = 1
    for j = 2:ny
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));
    end
end

% corners
j = 1;
fx(i,j) = (potential(i,j+1)-potential(i,j))/(rx(i,j));
fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));

j = nx+1;
fx(i,j) = (potential(i,j)-potential(i,j-1))/(rx(i,j));
fy(i,j) = (potential(i+1,j)-potential(i,j))/(ry(i,j));

% bottom
for i = ny+1 %last row
    for j = 2:nx % interior columns
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(1,j));
        fy(i,j) = (potential(i,j)-potential(i-1,j))/(ry(1,j));
    end
end
\begin{verbatim}
end

% corners
j = 1;
fx(i,j) = (potential(i,j+1)-potential(i,j))/(rx(i,j));
yf(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));

j = nx+1;
fx(i,j) = (potential(i,j)-potential(i,j-1))/(rx(i,j));
yf(i,j) = (potential(i,j)-potential(i-1,j))/(ry(i,j));

%% sides with Dirchlet bc
% left side
for i = 2:ny %interior for rows
    for j = [1 nx+1] % first and last column
        fy(i,j) = (potential(i+1,j)-potential(i-1,j))/(2*ry(i,j));
    end
end

%% Interior
for i = 2:nx
    for j = 2:ny
        fx(i,j) = (potential(i,j+1)-potential(i,j-1))/(2*rx(i,j));
        fy(i,j) = (potential(i+1,j)-potential(i-1,j))/(2*ry(i,j));
    end
end
\end{verbatim}
function f = VanderWaals_Casimir(Area,Ael_gate1,Ael_gate2,...
    gap,gap_gate1,gap_gate2,U,Uc_gate1,Uc_gate2,...
    nls,nls_gate1,nls_gate2,f,AnalysisType)

%%-----------------------------------------------------------------------
% Written By Bradley Darren Davidson 2010
% This program will compute the vdw and casimir force between deformed
% plates for NEMS devices
% Outputs: total load contribution from the interactions
%%-----------------------------------------------------------------------

%------------------------------------------------------------------------
% Important constants
%------------------------------------------------------------------------

A12 = 22e-12*(1e6)^2;   % Hamaker.

% hbar = 6.62608e-34/(2*pi);
% hbar = 0;       % nullify contribution from casimir
% c = 3e8;       % speed of light, for casimir forces,
% this is in m/s should be in micron per second!!!!!!!
%% Drain Electrode

switch AnalysisType
    case {10,11}
        fd = zeros(size(f));  fg1 = zeros(size(f));  fg2 = zeros(size(f));
        f_actuation = zeros(size(f));
        Load_actuation = zeros(size(f));

    end

%------------------------------------------------------------------
% Drain Loads
%------------------------------------------------------------------

% van der Waals load
for j = 1:length(nls)-1
    load_vdw(nls(j,1),2) = (-A12.*Area(j)./(6*pi*(gap+U(j,1)).^3));
end

% Casimir load
for j = 1:length(nls)-1
    load_casmir(nls(j,1),2)...
        = (-hbar.*Area(j).*pi.^2.*c./(240.*(gap+U(j,1)).^4));
end

%------------------------------------------------------------------
% Add loads
%------------------------------------------------------------------

dist_el = 2;
Load_actuation = (load_casmir+load_vdw)/dist_el;

%------------------------------------------------------------------
% Assemble Load vector
%------------------------------------------------------------------
j = 1;
for i = 1:length(nls)-1
    \( f_{\text{actuation}}(2nls(i,1)-1:2nls(i,1),j) = \text{Load}_{\text{actuation}}(nls(i,1),:) ; \)
    \( f_{\text{actuation}}(2nls(i+1,1)-1:2nls(i+1,1),j) = \text{Load}_{\text{actuation}}(nls(i,1),:) ; \)
    j = j+1;
end

fd = sum(f_{\text{actuation}}')' \times 1e6;
end

%% Left Gate Electrode
switch AnalysisType
    case 11
        f_{\text{actuation}} = zeros(size(f));
        load_vw = zeros(length(nls_{gate1})-1,2);
        load_casmir = zeros(length(nls_{gate1})-1,2);
        Load_{actuation} = zeros(size(f));

        % Gate 1 Loads
        for j = 1:length(nls_{gate1})-1
            load_vw(nls_{gate1}(j,1),2) = (-A12 \times Ael_{gate1}(j)/(6 \times \pi \times (gap_{gate1}+Uc_{gate1}(j))^3));
        end

        for j = 1:length(nls_{gate1})-1
            load_casmir(nls_{gate1}(j,1),2) = ...

        end
    end
end
\[
= (-\hbar \cdot A_{\text{el} \text{ gate1}}(j) \cdot \pi^2 \cdot c/(240 \cdot (\text{gap}_{\text{gate1}}+... \\
U_{\text{c\_gate1}}(j,1)).^4));
\]

end

%--------------------------------------------------------------------
% Add loads
%--------------------------------------------------------------------

dist_el = 2;
Load_actuation = (load_electro+load_casmir+load_vw)/dist_el;

%--------------------------------------------------------------------
% Assemble Load vector
%--------------------------------------------------------------------

j = 1;
for i = 1:length(nls_gate1)-1
    f_actuation(2\cdot nls_gate1(i,1)-1:2\cdot nls_gate1(i,1),j)...
        = Load_actuation(nls_gate1(i,1),:);

    f_actuation(2\cdot nls_gate1(i+1,1)-1:2\cdot nls_gate1(i+1,1),j)...
        = Load_actuation(nls_gate1(i,1),:);
    j = j+1;
end

f_1 = sum(f_actuation')*1e6;

%% Right Gate Electrode
f_actuation = zeros(size(f));
Load_actuation = zeros(size(f));
load_vw = zeros(length(nls_gate2)-1,2);
load_casmir = zeros(length(nls)-1,2);
% Gate 2 Loads

for j = 1:length(nls_gate2)-1
    load_vw(nls_gate2(j,1),2)...
        = (-A12.*Ael_gate2(j)./(6*pi*(gap_gate2+Uc_gate2(j,1)).^3));
end

for j = 1:length(nls_gate2)-1
    load_casmir(nls_gate2(j,1),2)...
        = (-hbar.*Ael_gate2(j)*pi.^2.*c./(240.*(gap_gate2...
            +Uc_gate2(j,1)).^4));
end

% Add loads

dist_el = 2;
Load_actuation = (load_casmir+load_vw)/dist_el;

% Assemble Load vector

j = 1;
for i = 1:length(nls_gate2)-1
    f_actuation(2*nls_gate2(i,1)-1:2*nls_gate2(i,1),j)...
        = Load_actuation(nls_gate2(i,1),:);
f_actuation(2*nls_gate2(i+1,1)-1:2*nls_gate2(i+1,1),j)...
    = Load_actuation(nls_gate2(i,1),:);
    j = j+1;
end

fg2 = sum(f_actuation')'*1e6;
end

%% Sum all Loads
switch AnalysisType
    case 11
        f_beam = fd+fg1+fg2;
        f_beam = sparse(f_beam)*1e-6; % scaling for VDW
    otherwise
        f_beam = fd;
        f_beam = sparse(f_beam)*1e-6; % scaling for VDW
end