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Steady and Unsteady Thermo-Strucural Simulation of Thermally Actuated Micro- and Nano-Structures

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STEADY AND UNSTEADY THERMO-STRUCTURAL SIMULATION
OF THERMALLY ACTUATED MICRO- AND NANO-STRUCTURES

A Dissertation

Submitted to the Graduate Faculty of the
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by

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ABSTRACT

This dissertation provides a thermo-structural simulation for nano-scale and micro-scale structures with pinned and fixed boundary conditions which are either thermally positioned, buckled, or actuated. The study begins with simulating a pinned-pinned beam in micro-scale and nano-scale. The steady state thermo-structural equation is solved numerically using an implicit Finite Difference method implemented in Matlab to obtain the thermal positioning response, which is the thermally steady state center displacement, by adding a constant, time-independent heat flux to the structure. The results show the steady state thermal displacement of the system is a function of the geometry, pressure, material properties, and constant heat flux in the free molecular model, while this value is independent of pressure in the continuum model. The thermal positioning simulation is used to improve the thermal efficiency of a thermal micro-switch by introducing various heating configurations.

The second thermal mode is thermal buckling which is used to introduce a new thermal buckling storage nano-memory. Using an unsteady simulation, the power requirements for thermal actuations, optimal geometry, and write time of the device for various materials are investigated. The results show that this memory consume a low power in the order of 1 nJ per bit and has a data storage density of $10^{11}$ bits/cm$^3$, which is acceptable in comparison with the current memory devices. Thermal buckling nano-memory is also radiation-protected, making it a good alternative for space exploration computer systems operating in high radiation and electromagnetic environments.

In contrast with thermal positioning and buckling, thermal actuation applies time-dependent heat load leading to vibration in the structure. An implicit Finite Difference method implemented in C++ was used to solve the coupled transient thermo-structural equations with
constant thermal properties, while an explicit approach was used to solve the variable properties thermo-structural equations. The response, the center displacement in a doubly-clamped bridge, is tracked by time and decomposed to the steady state and vibration amplitudes. The results show that constant thermal properties assumption is limited for small heat additions lower than 1 mW. Thermal actuation results are applicable in simulating the dynamic behavior of nano-scale devices used for switching, nano-manufacturing, and measurement.
CHAPTER 1: INTRODUCTION

1.1 Actuation Modes

Nano-Electro-Mechanical Systems, NEMS and Micro-Electro-Mechanical Systems, MEMS devices are actuated using several methods including electrostatic, thermal, mechanical and magnetic actuation. The response of these systems is the displacement of the structure. Figure 1.1 shows a micro-bridge and a micro-cantilever schematic. Both structures are actuated using a distributed force along the structure. The center displacement determines the response of the bridge structure. The tip displacement determines the response of the cantilever structure.

![Micro-bridge schematic](image1)

![Micro-cantilever schematic](image2)

Figure. 1.1 The actuation and response in NEMS and MEMS structures (a) Micro-bridge (b) Micro-cantilever

If the actuation force is created by heating, and creating thermal stresses within the structure, then the system is said to be thermally actuated. The term "thermal actuation" is commonly used to describe three related phenomenon. In the first case, a constant heat load is added to a system to change the static deflection of the system by changing the thermal stresses asymmetrically to adjust the displacement of the system. In the second case, a constant heat load is added to a system
to change the static deflection of the system by thermally buckling the system. In the third case, a time-dependent heat input is added to the system. This leads to time-dependent thermal stresses, and vibration, in the system.

To avoid ambiguity, the first case, changing the thermal stresses asymmetrically to adjust the displacement of the system, is referred to as "thermal positioning" and the second case, changing the thermal stresses asymmetrically to buckle the system, is called "thermal buckling". The term "thermal actuation" is left for the third case, time-dependent heat load and time-dependent response. Figure 1.2 shows the actuation modes categories.

The thermal response of the NEMS and MEMS devices determines the mechanical response of these systems. The displacement, which is the mechanical response, is determined by thermal stress. An example of this is thermal bimorph actuation applied for a Parallel Dip-pen Nanolithography (PDN) probe array (Wang et al., 2004). An adjustable dc voltage source was used to supply power to the actuators. The silicon DPN probe thermal displacement variation verses actuation power corresponds to a linear system. The maximum displacement of 28 μm was achieved at an actuation power of 17.57 mW, which is adequate to overcome the surface adhesion force.
1.1.1 Thermal Positioning

As explained in the introduction, thermal positioning refers to changing the static position of a micro- or nano-structure. In this case the thermal actuation is a steady constant heat load and not a function of time. The mechanical response of the system, which is defined as displacement is determined when the system reaches to thermally steady state.

This procedure can be applied to the phenomenon in which the study of the response by time is not important. For example, assume an open state of a thermal-switch is called position 1, and a closed state of it is called position 2. Thermal positioning can determine the switch thermal power consumption and the switch efficiency when it moves from position 1 to position 2. However, it is not capable of discussing how long it takes for the switch to move from position 1 to position 2 and any other time dependent terms such as opening time lag and etc.

1.1.2 Thermal Buckling

Thermal buckling occurs when the axial force due to thermal stress in the structure becomes equal to the critical buckling force. At this time, the structure is assumed buckled. The buckled structure remains in its position without requiring adding external heat or force.

Thermal buckling is a family of thermal positioning as shown in Figure 1.1. It also refers to changing the static position of a micro- or nano-structure specifically from an un-buckled position to a buckled position. The thermal actuation is a constant heat load. However, the response is a time dependent phenomenon. It has an application in buckling beam memory storages, which will be discussed later in chapter 5.

1.1.3 Thermal Actuation

While applying a constant heat load leads to static structural behavior, sinusoidal heating leads to vibration in the bridge. In thermal actuation, the heat load is not a constant. Instead, it is a
harmonic function of time. As a result, the structure response of the thermal actuation is time-independent.

In contrast with thermal positioning, thermal actuation captures the transient response of a thermal switch while it is changing position from open to close. Using the time-dependent response, the closing time and opening time (after stop heating the structure) can be determined. Figure 1.3 shows time-dependent excitation and response in a nano-scale resonator.

![Time-dependent excitation and response in a thermally actuated micro-structure](image)

Figure 1.3 Time-dependent excitation and response in a thermally actuated micro-structure

1.2 Applications

Thermally positioned and actuated micro and nano-scale structures have scientific and commercial applications, including wireless communication systems (Nguyen, 1999; Jensen et al., 2007) nano-scale fabrication, (Piner et al., 1999; Fan et al., 2000; Ding et al., 2010), data storage (Vettiger et al., 2002), and optical systems (Pal et al., 2009). MEMS and NEMS (Micro- and Nano-Electro-Mechanical Systems) devices have widths and lengths on the order of microns, and thicknesses on the order of 100 nanometers. These devices are either mechanically or thermally actuated. Laser beams thermally actuate devices in laboratory experiments, while electrical heaters
are proposed for general applications. The mechanical response of these systems is the displacement of the structure.

A variety of experiments have been conducted in thermally actuated devices with a constant heat load. These include the use of micro-scale electrical heaters and laser which control the temperature of photonic crystal devices. A method using a laser beam was reported by Faraon et al. (Faraon et al., 2007) to locally control the temperature of the photonic crystal by external heating. In a related study, Faraon and Vuckovic (Faraon and Vuckovic, 2009) used this method by applying electrical heaters to control the resonant frequency of InAs quantum dots coupled to GaAs photonic crystal resonators, enabling independent control of large ensembles of photonic devices at high tuning speeds. Zhu et al. (Zhu et al., 2011) integrated a novel electrothermal nano-positioner with an electrothermal actuator in the same MEMS chip without the need for inclusion of extra electrical insulation fabrication process or assembling two chips. The on-chip displacement sensing enables a feedback control capability. They also calibrated the nano-positioner by studying the displacement variations by the actuation voltage. Wang et al. (Wang et al., 2008) developed a wavelength-selective photonic switch using thermo-optic effects. They used a local micro-heater to tune the resonance wavelength to a target signal wavelength.

### 1.2.1 Nano- and Micro-Bridge Switches

There are several thermally actuated micro- and nano-devices such as switches and resonators. In thermal switching, an infrared laser beam was used by Hashimoto et al. (Hashimoto et al., 1994) to control the magnetic actuator. A spot-heating infrared laser heats one of the stators in the switch and reduces its magnetization. As a result, the force between the two stators changes and the other stator attracts the armature. Laser heating can also play a role as external excitation sources in bridge resonators (Svitelskiy et al., 2008).
Thermal-electrostatic micro-switches work based on displacement variation of the switch structure without using a movable thermal contact liquid. Carmona et al. modeled thermal actuation in a thermo-pneumatic micro-pump (Carmona et al., 2003). Thermal actuation increases the air temperature in this pump, generating the membrane deflection.

Thermal-electrostatic micro-switches result in a low actuation voltage but consume a high power. There are various types of thermal switches such as bridges, cantilevers, and lateral series of these two types (Rebeiz, 2003). Various numerical and experimental studies have been performed on different designs of micro-switches. Reid et al. simulated a cantilever micro-switch to investigate the effects of changes in the geometry on the operational range of the switch (Reid and Starman, 2003). Coutu et al. modeled a cantilever micro-switch pull-in voltage, collapse voltage, and contact force predictions, analytically. The results were compared with experimental results (Coutu et al., 2004). Dequenes et al. studied the pull-in voltage of several nanotube-based nano-switches including the bridges and cantilevers and proposed a continuum model for the simulation of carbon-nanotube-based NEMS switches (Dequenes et al., 2002).
Blondy et al. designed and fabricated a thermally actuated silicon nitride micro-switch bridge as shown in Figure 1.5. Experimental measurements showed that the switch has a low actuation voltage. The switch also offered high isolation, and mechanical protection (Blondy et al., 2001).

![Image of micro-switch bridge](image)

**Figure 1.5 The thermally actuated micro-switch designed by Blondy et al. (2001)**

Duong investigated the environmental conditions effects on the reliability of five different micro-switches. All models are categorized as bridge switches but with different geometrical designs. The actuation voltage and deflection variations versus temperature variations were studied using modeling and experimental tools. The switch dilation and pull-in voltage variations by temperature and temperature cycles were investigated (Duong et al., 2005).

### 1.2.2 Nano- and Micro-Bridge Memory

The concept of mechanical bistability of a doubly-clamped bridge was used to implement non-volatile electro-mechanical memory (Nagami et al., 2012) and volatile mechanical memory (Badzey et al., 2004) operating based on the displacement of the bridge. A potentially simpler non-volatile memory device is the buckled-beam nano-mechanical memory (Hälg et al., 1990; Roodenburg et al., 2009; Charlot et al., 2008). These devices have been electrostatically actuated. After the beam is buckled through application of an electrostatically generated force, the bistable beam remains buckled after the power is removed. These devices have been successfully demonstrated in laboratory experiments (Roodenburg et al., 2009), but have not been the subject of extensive performance or reliability analysis.
The buckling-beam concept was also used in fabrication of other devices such as snapping membranes which are used as temperature indicators. These devices are thermally actuated and buckle downward with an increase in temperature beyond a critical value. Just as in electrostatically actuated devices, they remain in the downward buckled state as the temperature decreases back to its initial value (Arya et al., 2006).

### 1.3 Actuation Physics

Because these devices are thermally actuated, the heat transfer equation in the system is a controlling parameter. Because the length and the width of the structure are in the micro scale and the thickness is in the order of hundreds of nanometer, the continuum conductive heat transfer equation can be used inside the device. Both continuum and free molecular regime were studied for convective heat transfer depending on the air pressure. The dimensionless Knudsen number determines which convective heat transfer coefficient must be used in the simulations as shown in Figure. 1.6. The Knudsen number is given by:

\[ Kn_L = \frac{\lambda}{L}, \]

where \( \lambda \) is the mean free path of the gas and \( L \) is the length scale of the beam. The mean free path is given by (Kennard, 1983):

\[ \lambda = \frac{1}{\sqrt{2\pi n d_g^2}}, \]

where \( n \) is the density of particles per volume, \( d_g \) is the collision diameter of the gas molecule.

The Knudsen number determines if continuum formulations of the momentum and energy equations are appropriate to use. As shown in Figure. 1.6, for Knudsen numbers more than 10 a free molecular heat transfer coefficient is valid. However, for Knudsen numbers less than 0.1, continuum heat transfer coefficient is valid.
The ambient pressure will change the Knudsen number and as a result, the flow regime. Lee et al. studied the thermal characteristics of a heated microcantilever considering conjugate heat transfer, conduction in the structure and convection between the structure and air or helium for a range of pressures (Lee et al., 2007). They showed for Kn>1, thermal transport from the cantilever heater is gas pressure dependent while for Kn<1, it remains constant. The continuum breaks down for Kn numbers more than 1, affects the convection between the cooling gas and the NEMS and MEMS devices which is an important parameter affecting the mechanical response of the system.

A method was presented to optimize a rectangular two-beam micro-electro-mechanical thermal actuator using a simplified heat transfer mechanism including convection (Hickey et al., 2002). They investigated buckling deflection due to thermal stress at uniform temperature, and presented the measurement of the deflection as a function of actuation voltage. Phinney et al. (Phinney et al., 2010) studied the effects of the pressure of the surrounding gas on the thermal performance of silicon bridges 10 μm wide, 2.25 μm thick and 200 to 400 μm long. They measured the temperature profile experimentally, in a nitrogen atmosphere. The numerical results obtained using a FEM (Finite Element Method) were compared with the experimental results. Their results show that gas phase heat transfer is an important parameter for devices of this size at ambient pressure. As the pressure decreases below 5 Torr, the effects of convection become minimal. Heat transfer in package MEMS was studied numerically using the Direct Simulation Monte Carlo method by Liu
et al. (Liu et al., 2007). The package was assumed as an enclosure with a hot chip at the bottom. The results showed if the bottom temperature was partly uniform at the center the heat transfer on the hot chip surface was enhanced comparing with the uniform temperature bottom case. Martin and Houston (Martin and Houston, 2009) characterized high frequency vibrating cantilever and bridge structures below the continuum limit. A net free molecular heat transfer for the system was calculated.

Several researchers have studied conductive heat transfer effects on the mechanical response of the system. Ilic et al. (Ilic et al., 2010) investigated the energy transport mechanisms in silicon nano-cantilevers experimentally. A modulated laser beam added thermal energy along the device layer. The thermal response of the device was obtained for unsteady thermal actuators in the absence of convection. Mastropaolo and Cheung (Mastropaolo and Cheung, 2008) studied the thermo-mechanical behavior of silicon carbide clamped-clamped bridges resonators. The simulations were performed for different electrode lengths, widths, and spacings to investigate the geometry effects on the mechanical response of the system. In a related study, Mastropaolo et al. (Mastropaolo et al., 2009) designed the electro-thermally actuated silicon carbide ring resonators to achieve higher resonant frequency compared to beam resonators. The double electrode configuration was found to be the most efficient design for actuation with a relatively high average temperature and the largest heated area.

1.4 Dissertation Organization

The thermo-structural equations are derived in chapter 2. This chapter begins with the derivation of unsteady heat transfer equation for both constant and variable thermal properties with and without thermo-elastic terms. The unsteady structural equation is derived using the equation of motion for an infinitesimal element on the beam and Bernoulli beam assumption. The structural equations boundary conditions are shown for both pinned-pinned and fixed-fixed ends conditions.
Chapters 3 and 4 focus on thermal positioning of micro- and nano-structures. A three-dimensional pinned-pinned micro- and nano-bridge is simulated in chapter 3. The steady response of the system with steady actuation (constant heat load) is discussed in this chapter to present a universal scaling for the behavior of micro- and nano-scale bridge structures over a range of dimensions (micro-scale to nano-scale), materials (silicon, silicon carbide and CVD diamond), ambient heat transfer conditions (free molecular and continuum approaches), and heat loads. The heat conduction equation is solved numerically using a Finite Difference method implemented in Matlab to obtain the temperature distribution in the bridge. Using the nodal temperature distribution, thermal stress due to the temperature difference with respect to the wall temperature is calculated. The structural equation is solved numerically to get the displacement along the beam. The algorithm and details of time domain and space domain discretization methods are discussed in details in chapter 3. The results are non-dimensionalized to provide insight into thermal positioning across a range of structure length scales and material properties. In addition, the continuum level effects are scaled with the statistical mechanics effects.

Chapter 4 uses the Finite Difference method which is presented in chapter 3 to solve the thermo-structural equations, to obtain closing power consumption and thermal efficiency of a thermally actuated bridge micro-switch for various heating configurations. Ideally, switch opening and closing times should be calculated through the full dynamic simulation. However, the steady state approach, with simpler structural and heat equations, is used in this study to estimate the efficiency and power consumption. Three heating configurations are used: distributed heat at the top surface, concentrated heat at the center of the top surface, and concentrated heat at the sides of the top surface. At time t=0, a constant heat load, q, is applied to the top of the bridge until the bridge reaches to a thermally steady state condition. The heating procedure is also performed for
closed-switch models with different thermal boundary conditions. Simulations are performed for two different materials: silicon and silicon nitride.

Chapter 5 applies the two technologies of buckling beam and thermal excitation to design a storage memory. In this work, a unit bridge of an array of buckling-beam memory is simulated using the Finite Difference method presented in chapter 3. The geometry and boundary conditions of the unit bridge are comparable with the geometry presented in chapter 3. The thermal boundary conditions are identical while the structural boundary conditions are changed to fixed-fixed boundary conditions. The heat load is preserved steady and constant; however, transient response to constant heating is studied to estimate the power requirements for thermal actuations, optimal geometry, and write time of the device for various materials.

In contrary with constant heat load excitation, applying sinusoidal heating leads to vibration in the bridge. Chapter 6 discusses the harmonic response of the thermally actuated doubly clamped nano-bridge to harmonic actuation. The heat load is defined as a sinusoidal harmonic actuation. An implicit Finite Difference solver implemented in C++ was used to solve the thermo-structural equations with constant thermal properties while an implicit Finite Difference method was used for temperature dependent thermal properties. The significance of temperature dependent thermal properties with the heat amplitude is studied. The phase delay between the excitation and the response and the amplitude of the response are investigated by various actuation frequencies at the pressure lower than atmospheric pressure.
CHAPTER 2: THREE DIMENSIONAL STEADY AND UNSTEADY GOVERNING THERMO-STRUCTURAL EQUATIONS

This chapter discusses the derivations of the governing equation in details for two different boundary conditions of a pinned-pinned bridge and a fixed-fixed bridge.

2.1 Geometry and Boundary Conditions

The study in this dissertation is performed on a micro- and nano-bridge structure with pinned-pinned boundary conditions for steady thermo-structural simulation as will be used in chapters 3 and 4. The boundary conditions are changed to fixed-fixed for unsteady thermo-structural simulation as will be discussed in chapter 6.

Figure 2.1 shows the thermal boundary condition in the bridge which is identical in the dissertation. The heat transfer includes conduction within the beam as well as convection between the beam and the quiescent gas are considered. The heat addition is modeled as a constant heat load, $q''$, applied to the top surface of the beam for the steady case as will be discussed in chapters 3 and 4 while the heat addition changes to harmonic heat load for the unsteady study as will be discussed in chapter 6.

The cooling gas is air with constant properties at ambient temperature. Various materials are used such as crystalline silicon, silicon carbide, and CVD diamond. The thermal properties of all materials are assumed to be constant and defined at the wall temperature. The wall temperature, $T_w$, is fixed at both ends of the beam.
2.2 Transient Heat Transfer Equation

The full three-dimensional transient heat conduction equation for constant thermal properties is given as follows (Incropera et al., 2007):

\[
\frac{\partial T(x, y, z, t)}{\partial t} = \frac{k}{\rho c_p} \left( \frac{\partial^2 T(x, y, z, t)}{\partial x^2} + \frac{\partial^2 T(x, y, z, t)}{\partial y^2} + \frac{\partial^2 T(x, y, z, t)}{\partial z^2} \right),
\]

(2.1)

where \( k \) is the thermal conductivity of the solid. This equation is solved using an implicit Finite Difference approach at each time step to obtain the nodal temperature distribution when the thermal properties are assumed constant at the wall temperature. This equation is used in the steady study in chapters 3 and 4.

However, the transient heat transfer equation is modified in order to take into account the thermo-elastic terms and also temperature dependency of the thermal properties. Adding the heat equation to the equation of motion yields the following equation (Landau and Lifshitz, 1959; Lifshitz and Roukes, 1999; Serra and Bonaldi, 2008):

\[
\frac{\partial T(x, y, z, t)}{\partial t} = \frac{1}{\rho c_p} \left( \frac{\partial}{\partial x} \left( k \frac{\partial T(x, y, z, t)}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T(x, y, z, t)}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T(x, y, z, t)}{\partial z} \right) \right) - \frac{E\alpha T}{(1-2\nu_p)c_v} \frac{\partial}{\partial t} \sum_f \varepsilon_{yy},
\]

(2.2)

where \( \nu_p \) is the poisson ratio and \( c_v \) is the specific heat per unit volume. \( \varepsilon_{yy} \) is the strain in the normal direction in all three directions. Using Hookes’ law, the strain components are defined as follows (Lifshitz and Roukes, 1999):

\[
\varepsilon_{xx} = \frac{\sigma_{xx}}{E} + \alpha(T - T_w),
\]

(2.3)

\[
\varepsilon_{zz} = \varepsilon_{yy} = -\nu_p \frac{\sigma_{xx}}{E} + \alpha(T - T_w),
\]

(2.4)

where \( \sigma_{xx} \) is the normal stress along the x axis due to bending. The second terms in the right hand side of Eqs. (2.3) and (2.4) represents the strain due to heat expansion.
The longitudinal normal strain of any element within the beam depends on its location \( z \) on the cross section and the radius of curvature of the beam's longitudinal axis at that point as shown in Figure 2.2:

\[
\varepsilon_{\text{ax}} = \varepsilon_x - \frac{z}{R_c},
\]

(2.5)

where \( \varepsilon_x^- \) is the strain at the bar middle surface:

\[
\varepsilon_x^- = \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right]
\]

(2.6)

where \( u \) is the axial displacement and \( v \) is the transverse displacement. Assuming pure transverse motion in the \( z \) direction, and making the usual Euler-Bernoulli assumption that the transverse dimensions of the beam are sufficiently small compared with the length and the radius of curvature \( R_c \), that any plane cross section, initially perpendicular to the axis of the beam, remains plane and perpendicular to the neutral surface during bending. As a result, \( \varepsilon_x^- \) is assumed negligible in comparison with the other terms. The curvature equation from calculus is:

\[
R_c = \frac{d^2 z}{dx^2} \left[ 1 + \left( \frac{dz}{dx} \right)^2 \right]^{\frac{3}{2}},
\]

(2.7)

Figure 2.2 The radius of curvature in a deformed element
which for actual beams can be simplified because the slope $dz/dx$ is small. The square is even smaller, and can be neglected as a higher order term. Taking into account this simplification, Eq. (2.7) becomes:

$$R_c = \frac{d^2z}{dx^2}. \quad (2.8)$$

Combining Eqs. (2.3), (2.5) and (2.8), the following expression is obtained for the normal stress due to bending:

$$\frac{\sigma_{zz}}{E} = -z \frac{\partial^2 \nu(x,t)}{\partial x^2} - \alpha (T - T_w). \quad (2.9)$$

Substituting Eq. (2.9) to Eq. (2.4), the normal strains in $z$ and $y$ directions become:

$$\varepsilon_{zz} = \varepsilon_{yy} = \nu_p z \frac{\partial^2 \nu(x,t)}{\partial x^2} + (1 + \nu_p) \alpha (T - T_w). \quad (2.10)$$

Substituting Eqs. (2.5) and (2.10) in Eq. (2.2), the finalized transient heat transfer equation including thermo-elastic terms and temperature dependent thermal properties, is obtained as follows:

$$\left(1 + \frac{2E\alpha c^2}{\rho c_p} \frac{T(x,y,z,t)}{1 - 2\nu_p} \right) \frac{\partial T(x,y,z,t)}{\partial t} =$$

$$\frac{1}{\rho c_p} \left( \frac{\partial}{\partial x} \left( k \frac{\partial T(x,y,z,t)}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T(x,y,z,t)}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T(x,y,z,t)}{\partial z} \right) \right)$$

$$+ \frac{E\alpha T(x,y,z)}{\rho c_p} \frac{\partial}{\partial t} \left( z \frac{\partial^2 \nu(x,t)}{\partial x^2} \right) \quad (2.11)$$

Equation (2.11) allows the incorporation of thermal properties as temperature dependent variables, and takes into account the thermo-elastic terms. This equation is solved using an explicit Finite Difference approach to obtain the nodal temperature distribution at each time step in chapter 6 for the study of the unsteady thermo-structural behavior.
2.3 Thermal Boundary Condition

The thermal boundary conditions are identical in this study from chapter 3 to chapter 6. There are three different types of boundary condition in this model as shown in Figure 2.1. The Dirichlet boundary condition at both ends is expressed as

\[ T = T_w. \]  \hspace{1cm} (2.12)

There are two different types of Neumann boundary conditions which are applied to the heated and unheated surfaces. Equation (2.13) shows the boundary condition for the heated surface, and Eq. (2.14) shows the boundary condition for the unheated surfaces:

\[ -k \frac{\partial T}{\partial n} = h(T - T_a) + q'', \]  \hspace{1cm} (2.13)

\[ -k \frac{\partial T}{\partial n} = h(T - T_u), \]  \hspace{1cm} (2.14)

2.4 Heat Transfer Coefficient

There are two different approaches to computing the heat transfer coefficient, \( h \). The selected method depends on the Knudsen number. The Knudsen number is defined as

\[ Kn_w = \frac{\lambda}{W}, \]  \hspace{1cm} (2.15)

where \( \lambda \) is the mean free path of the gas and \( W \) is the width scale of the beam. For a dilute gas assumption, the molecular mean free path is given by

\[ \lambda = \frac{k_b T_a}{\sqrt{2 \pi P_{\text{gas}} d_g^2}}, \]  \hspace{1cm} (2.16)

where \( k_b \) is the Boltzmann constant, \( T_a \) is the ambient temperature, \( P_{\text{gas}} \) is the pressure of the gas, and \( d_g \) is the effective diameter of the gas molecule (Lee et al., 2007). The molecular collisions between the beam and the gaseous medium decreases as Knudsen number approaches 1. The heat transfer coefficient in a gas with the Knudsen number more than 1 will be (Martin et al., 2009):
\[ h = \sigma_T n_i \left( \gamma + 1 \right) \sqrt{\frac{k_b \gamma T_a}{8\pi m}} \]  
\hspace{1cm} (2.17)

where \( \sigma_T \) is the thermal accommodation coefficient, \( \gamma \) is the specific heat ratio of the gas, \( m \) is the molecular weight of the gas, and \( n_i \) is the number density of the gas. For an ideal gas, \( n_i \) can be calculated using

\[ n_i = \frac{P_{\text{gas}}}{m RT_a} \]  
\hspace{1cm} (2.18)

where \( R \) is the ideal gas constant.

The continuum theory is valid for a Knudsen number less than 0.01. If the air is quiescent, the heat transfer from the structure can be modeled as conduction into an infinite medium. This can be treated as an effective value of the heat transfer coefficient, \( h \):

\[ h = q_{ss}^* k_{\text{gas}} \sqrt{\frac{2\pi}{WL}} \]  
\hspace{1cm} (2.19)

where \( q_{ss}^* \) is the steady-state dimensionless conduction heat rate, \( k_{\text{gas}} \) is the conductivity of the gas, and \( W \) and \( L \) are the width and the length of the beam, respectively. For an infinitely thin rectangle of length \( L \), width \( W \), and constant temperature in an infinite medium of constant temperature, \( q_{ss}^* \) is estimated as 0.932 (Incropera et al., 2007).

In the transition region, where the Knudsen number is between 0.01 and 1, it is computationally difficult to estimate the heat transfer coefficient. In this study, the results in this region are assumed to fall between the molecular and continuum results.

Previous researchers studied the heat transfer coefficient as a function of pressure (Lee et al., 2007; Park et al., 2007; Ramanan and Yang, 2009; Narayanaswamy and Gu, 2011). A combined computational and experimental study of the heat transfer from a micro-heater modeled a micro-cantilever beam by employing the thermal resistance network. At low pressures, the convective
heat transfer coefficient is a function of pressure, as expected from free-molecular theory. As the pressure passes 40 kPa, heat transfer coefficient goes to a constant value of 1250 W/m²K (Lee et al., 2007). This suggests that a continuum condition has been reached. In order to validate Eq. (2.19), heat transfer coefficient is calculated for the length of 100 μm, and the width of 10 μm. Eq. (2.19) will give a value of 1890 W/m²K, suggesting it is a reliable order-of-magnitude approximation.

2.5 Transient Structural Equation

In order to derive the transient structural equation, equation of motion for an infinitesimal element with the length dx on a Bernoulli beam shown in Figure 2.3 is derived.

![Figure 2.3 Infinitesimal element on a Bernoulli beam](image)

Figure 2.4 shows the forces acting on the element. Figure 2.4 (see a) shows the shear force variation along the element. The equation of motion in this case will be as follows:

$$\rho A \frac{\partial^2 \nu(x,t)}{\partial t^2} = \frac{\partial V}{\partial x}.$$  

(2.20)

Assuming the shear force does not change along the element as no external force is acting on the beam and only the bending moment due to heating the system changes along the element, as shown in Figure 2.4 (see b), the balance of force and momentum gives:

$$V = \frac{\partial M}{\partial x}.$$  

(2.21)
Combining Eqs. (2.20) and (2.21), the equation of motion is obtained as follows:

\[ \rho A \frac{\partial^2 v(x,t)}{\partial t^2} = \frac{\partial^2 M}{\partial x^2}, \]  

(2.22)

where M is the net moment representing the moment due to the mechanical deflection and the moment due to the thermal excitation. Taking into account the compression axial force in the system, Eq. (2.22) changes as follows (Jones, 2006):

\[ \rho A \frac{\partial^2 v(x,t)}{\partial t^2} + N \frac{\partial^2 v(x,t)}{\partial x^2} - \frac{\partial^2 M(x,t)}{\partial x^2} = 0, \]  

(2.23)

where N is the axial force in the beam. Bending moment and axial force can be obtained using the axial stress given in Eq. (2.3). Bending moment is calculated by integrating the axial stress over each plane:

\[
M(x,t) = \int \sigma_{xx} z dA \\
= E \int (\varepsilon_{xx} - \alpha(T - T_w)) z dA \\
= E \int \left( \varepsilon_x - z \frac{\partial^2 v}{\partial x^2} - \alpha(T - T_w) \right) z dA \\
= E \int \varepsilon_x z dA - E \int z \frac{\partial^2 v}{\partial x^2} z dA - E \int \alpha(T - T_w) z dA,
\]  

(2.24)

where \( \varepsilon_x \) does not vary over the bar cross-sectional area because the origin is at the centroid. As a result the first integral term in the last line is zero. The bending moment can be written as:
\[ M(x,t) = -EI \frac{\partial^3 v}{\partial x^2} - E \int \alpha(T - T_w) dA, \]  
\[ = -EI \frac{\partial^3 v}{\partial x^2} - M_{th}, \]  
\hspace{1cm} (2.25)\]

where \( M_{th} \) is the thermal bending moment and \( I \) is the moment of inertia:

\[ I = \int z^2 dA \]
\[ = \int z^2 y dz = \frac{W d^3}{12}. \]  
\hspace{1cm} (2.26)\]

The calculated bending moment shown in Eq. (2.25), includes the mechanical bending moment term and thermal bending moment. The axial force \( N \) is calculated using the axial stress given in Eq. (2.3):

\[ N(x,t) = \int \sigma_y dA \]
\[ = E \int (\varepsilon_{xy} - \alpha(T - T_w)) dA \]
\[ = E \int \left( \varepsilon_z - z \frac{\partial^2 v}{\partial x^2} - \alpha(T - T_w) \right) dA \]
\[ = E \int \varepsilon_z dA - E \int z \frac{\partial^2 v}{\partial x^2} dA - E \int \alpha(T - T_w) dA, \]  
\hspace{1cm} (2.27)\]

where the second integral in the last line is zero because the first moment of area is zero at the centroidal axis. Using Eq. (2.6), Eq. (2.27) can be rewritten as follows:

\[ N(x,t) = EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right] - E \int \alpha(T - T_w) dA \]
\[ = EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right] - N_{th}, \]  
\hspace{1cm} (2.28)\]

where \( N_{th} \) is the thermal compression force. Substituting Eqs. (2.25) and (2.28) in Eq. (2.23) and adding the damping term, the transient structural equation becomes:

\[ \rho A \frac{\partial^2 v(x,t)}{\partial t^2} + \left( EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right] - N_{th} \right) \frac{\partial^2 v(x,t)}{\partial x^2} + \frac{\partial}{\partial x} \left( EI \frac{\partial^2 v(x,t)}{\partial x^2} + M_{th} \right) + F_D(x,t) = 0, \]  
\hspace{1cm} (2.29)\]
where the damping term, $F_D$ is the net flow drag (Martin and Houston, 2008) in the free molecular regime. It is equivalent with the constant damping term, $C_f$ multiplied by vibration velocity. $F_D$ is given by:

$$F_D = \frac{W_p}{c}U(x,t) \left[ (2 - \sigma_n)\left(\frac{2}{\sqrt{\pi}} + 1\right) + \sigma_n\sqrt{\pi} \frac{T_w}{T_a} + 2 \frac{d}{W} \frac{\sigma_t}{\sqrt{\pi}} \right] = C_f U(x,t),$$

(2.30)

where $\sigma_n$, normal accommodation coefficient and $\sigma_t$, tangential accommodation coefficient are assumed to be equal to 1. The thermal velocity, $c$, is defined in Eq. (2.31), and $U(x,t)$ is the velocity in the vibration direction, $z$ which is defined as Eq. (2.32).

$$c = \sqrt{\frac{2k_bT_a}{m}},$$

(2.31)

$$U(x,t) = \frac{\partial v(x,t)}{\partial t},$$

(2.32)

where $m$ is the mass of the gas molecules, in this case air with $m=481.1 \times 10^{-27}$ kg. Other terms, $k_b$ and $T_a$ are previously defined as Boltzmann constant and ambient temperature.

Substituting Eqs. (2.30) in Eq. (2.29), the finalized dynamic structural equation is obtained:

$$\rho A \frac{\partial^2 v(x,t)}{\partial t^2} + \left( EA \frac{\partial u}{\partial x} + \frac{1}{2} \frac{\partial ^2 v}{\partial x^2} \right) - E \int \alpha (T - T_w) dy dz \frac{\partial^2 v(x,t)}{\partial x^2}$$

$$+ \frac{\partial}{\partial x} \left( EI \frac{\partial^2 v(x,t)}{\partial x^2} + E \int \alpha (T - T_w) dz dy \right) + C_f \frac{\partial v(x,t)}{\partial t} = 0.$$

(2.33)

The above equation is used in chapter 6 to study the dynamic behavior of a beam with fixed-fixed boundary conditions. A sensitivity study in chapter 6 will show that the axial force and the strain at the bar middle surface can be ignored in comparison with the bending moment.

For pinned-pinned boundary conditions where the bending moment is zero at the supports, the steady structural equation can be written as follows:

$$EI \frac{\partial^2 v(x,t)}{\partial x^2} + M_n = 0.$$

(2.34)
Equation (2.34) is used in chapters 3 and 4 to study the steady thermo-structural behavior of a bridge with pinned-pinned boundary conditions.

2.6 Structural Boundary Conditions

The bending moment is zero at the supports for pinned-pinned boundary conditions which is used in chapters 3 and 4. In this case, equation (2.34) is numerically solved using a Finite Difference method. The following boundary conditions is applied to the both ends where the moment is zero at the both ends:

\begin{equation}
\nu(x = 0, L) = 0. \tag{2.35}
\end{equation}

In chapter 6 dynamic structural equation Eq. (2.33) is solved for a fixed-fixed bridge to study the unsteady thermo-structural behavior of the structure. In this case, slope zero and displacement zero boundary conditions are applied at the both ends:

\begin{equation}
\begin{aligned}
\nu(x = 0, L, t) &= 0, \\
\frac{\partial \nu}{\partial x}(x = 0, L, t) &= 0. \\
\end{aligned} \tag{2.36}
\end{equation}
CHAPTER 3: THREE DIMENSIONAL SIMULATION OF STEADY STATE HEAT TRANSFER IN MICRO- AND NANO-BRIDGES

While applying sinusoidal heating leads to vibration in the bridge, a constant heat load leads to static structural displacement. This chapter simulates a 3-dimensional pinned-pinned bridge in micro and nano-scales to obtain a universal scaling for the behavior of micro- and nano-scale bridge structures. A Finite Difference method implemented in Matlab was used to solve the thermo-structural equations numerically. Simulations are performed over a range of dimensions, materials, ambient heat transfer conditions, and constant heat loads. This chapter performs this study for three different materials: silicon, silicon carbide and CVD diamond. Both free molecular and continuum approaches are used to define the heat transfer coefficient. The results are non-dimensionalized to provide insight into thermal positioning across a range of structure length scales and material properties. In addition, the continuum level effects are scaled with the statistical mechanics effects.

This chapter analyzes changing the thermal stresses asymmetrically to adjust the displacement of the system. To avoid ambiguity, this process will be referred to as "thermal positioning" instead of "thermal actuation."

3.1 Geometry and Boundary Conditions

The study uses two geometries: one pinned-pinned beam with a length L, of 100 microns, a width W, of 10 microns, and a thickness d, of 3 microns, and a second beam with a length of 10 microns, a width of 1 micron, and a thickness of 300 nanometers. The heat transfer and structural equations are solved numerically using a finite-difference method. Conduction within the beam as well as convection between the beam and the quiescent gas are considered. The heat addition is modeled as a constant heat load, q', applied to the top surface of the beam. This also corresponds
to the heat addition of a thin resistive film. Figure 3.1 shows the geometry and boundary conditions of the model.

![Figure 3.1 The geometry and boundary conditions in the model](image)

The cooling gas is air with constant properties at ambient temperature. Simulations are performed for three different materials: crystalline silicon, silicon carbide, and CVD diamond. The thermal properties of all materials are assumed to be constant and defined at the wall temperature. The wall temperature, $T_w$, is fixed at both ends of the beam.

### 3.2 Thermo-structural Formulation

#### 3.2.1 Heat Transfer Coefficient

There are two different approaches to computing the heat transfer coefficient, $h$. The appropriate method depends on the Knudsen number. The Knudsen number is defined as

$$Kn_w = \frac{\lambda}{W},$$

where $\lambda$ is the mean free path of the gas and $W$ is the width scale of the beam. For a dilute gas assumption, the molecular mean free path is given by

$$\lambda = \frac{k_b T_a}{\sqrt{2 \pi P_{\text{gas}} d_g^2}},$$

where $k_b$ is the Boltzmann constant, $T_a$ is the ambient temperature, $P_{\text{gas}}$ is the pressure of the gas, and $d_g$ is the effective diameter of the gas molecule (Lee et al., 2007). The molecular collisions between the beam and the gaseous medium decreases as Knudsen number approaches 1. The heat transfer coefficient in a gas with the Knudsen number more than 1 will be (Martin et al., 2009):
\[ h = \sigma_T n_i \frac{\gamma + 1}{\gamma - 1} \frac{k_b T_a}{8\pi m}, \]  

where \( \sigma_T \) is the thermal accommodation coefficient, \( \gamma \) is the specific heat ratio of the gas, \( m \) is the molecular weight of the gas, and \( n_i \) is the number density of the gas. For an ideal gas, \( n_i \) can be calculated using

\[ n_i = \frac{P_{\text{gas}}}{m RT_a}, \]

where \( R \) is the ideal gas constant.

The continuum theory is valid for a Knudsen number less than 0.01. If the air is quiescent, the heat transfer from the structure can be modeled as conduction into an infinite medium. This can be treated as an effective value of the heat transfer coefficient, \( h \):

\[ h = q_{ss}^* k_{\text{gas}} \frac{2\pi}{WL}, \]

where \( q_{ss}^* \) is the steady-state dimensionless conduction heat rate, \( k_{\text{gas}} \) is the conductivity of the gas, and \( w \) and \( l \) are the width and the length of the beam, respectively. For an infinitely thin rectangle of length \( L \), width \( W \), and constant temperature in an infinite medium of constant temperature, \( q_{ss}^* \) is estimated as 0.932 (Incropera et al., 2007).

In the transition region, where the Knudsen number is between 0.01 and 1, it is computationally difficult to estimate the heat transfer coefficient. In this study, the results in this region are assumed to fall between the molecular and continuum results.

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heat transfer coefficient is a function of pressure, as expected from free-molecular theory. As the pressure passes 40 kPa, heat transfer coefficient goes to a constant value of 1250 W/m2K (Lee et al., 2007). This suggests that a continuum condition has been reached. In order to validate Eq. (2.19), heat transfer coefficient is calculated for the length of 100 μm, and the width of 10 μm. Eq. (2.19) will give a value of 1890 W/m²K, suggesting it is a reliable order-of-magnitude approximation.

3.2.2 Governing Equations

In the current work, the full 3-dimensional steady heat conduction equation, Eq. (3.1), which is the steady state form of Eq. (2.1), is solved numerically to obtain the temperature distribution:

\[ k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = 0, \]

where \( k \) is the thermal conductivity of the solid.

There are three different types of boundary condition in this model (Figure 3.1). The Dirichlet boundary condition at both ends is expressed as

\[ T = T_w. \]

(2.12)

There are two different types of Neumann boundary conditions which are applied to the heated and unheated surfaces. Eq. (2.13) shows the boundary condition for the heated surface, and Eq. (2.14) shows the boundary condition for the unheated surfaces:

\[ -k \frac{\partial T}{\partial n} = h(T - T_a) + q", \]

(2.13)

\[ -k \frac{\partial T}{\partial n} = h(T - T_a) \]

(2.14)

The heat conduction equation is solved numerically using a finite difference method (Incropera et al., 2007). As a result, the temperature is obtained at each node. These results are used to calculate the thermal moment due to thermal stresses as previously shown in Eq. (2.25):
\( M_m(x, t) = E \int \alpha(T - T_w) z \, dA. \)  

(3.2)

In order to obtain the displacement distribution along the beam, Eq. (2.34) is numerically solved using a finite difference method.

\[ EI \frac{\partial^2 v(x, t)}{\partial x^2} + M_m = 0. \]  

(2.34)

The moment and displacement are zero at both ends for pinned-pinned boundary condition:

\[ v(x = 0, L) = 0. \]  

(2.35)

For small temperature variations, the modulus of elasticity, \( E \), is a constant.

### 3.2.3 Discretization and Algorithm

In order to solve the system of equations numerically using a Finite Difference method, the domain is discretized uniformly in the \( x, y \) and \( z \) directions. The grid spacing is called \( \delta_x \), \( \delta_y \) and \( \delta_z \).

The study of thermal behavior of the system is performed by solving the transient form of Eq. (3.1). The solution is performed iteratively until the thermally steady state solution is obtained. The temperature difference between two consecutive iterations is defined as a root mean square error. As soon as this error becomes smaller than the tolerance the system is assumed thermally steady state.

A central Finite Difference method is used for spatial implementation and unconditionally stable fully implicit scheme is used for time implementation (Patankar, 1980). An explicit time discretization scheme can be used alternatively to avoid the complications of matrix inversion methods in solving the discretized system of equations. However, in this scheme the time step \( \delta t \) must be small enough to satisfy the stability conditions of:

\[ \delta t < \frac{\rho c \delta x^2}{2k}. \]  

(3.3)
\[ \delta t < \frac{\rho c \delta^2}{2k} . \]  (3.4)

\[ \delta t < \frac{\rho c \delta^2}{2k} . \]  (3.5)

In this problem the grid spacing \( \delta_x \), \( \delta_y \) and \( \delta_z \) are in the order of nanometer. This requires the time step, \( \delta t \) to be at most in the order of \( 10^{-12} \) second to satisfy the stability condition. This increases the computation time to obtain the steady state results. However, the implicit scheme is unconditionally stable and independent of time step. As a result, an implicit scheme is selected to reduce the computation time and obtain the result faster.

### 3.2.3.1. Discretized Equations.

The number of boundaries determines the number of discretized equations are needed to solve this problem using Eqs (2.12) to (2.14).

Equation (3.6) shows the discretized transient form of Eq. (2.1) for the interior nodes (all nodes except the boundaries):

\[
T_{i,j,k}^n = \left(1 + 2Fo_x + 2Fo_y + 2Fo_z \right) T_{i,j,k}^{n+1} - Fo_x \left(T_{i-1,j,k}^{n+1} + T_{i+1,j,k}^{n+1} \right)
- Fo_y \left(T_{i,j-1,k}^{n+1} + T_{i,j+1,k}^{n+1} \right) - Fo_z \left(T_{i,j,k-1}^{n+1} + T_{i,j,k+1}^{n+1} \right),
\]  (3.6)

where \( i, j, \) and \( k \) determine the location of discretized temperature values in the \( x, y, \) and \( z \) axis respectively. The current time step is determined by \( n \) and the next time step is determined by \( n+1 \).

\( Fo \) is non-dimensional Fourier number defined as following in each direction:

\[
Fo_x = \frac{k \delta t}{\rho c (\delta x)^2}, \]  (3.7)

\[
Fo_y = \frac{k \delta t}{\rho c (\delta y)^2}, \]  (3.8)

\[
Fo_z = \frac{k \delta t}{\rho c (\delta z)^2}. \]  (3.9)
Equation (2.13) results in three discretized equations for the top heated surface and lines which are used for the nodes on: the top heated surface, the front top line, and the back top line. Equation (3.10) shows the discretized equation for the nodes located on the top heated surface:

\[
T_{i,j,p}^n = \left( 1 + 2Fo_x + 2Fo_y + 2Fo_z + 2Bi_zFo_z \right) T_{i,j,p}^{n+1} - Fo_x \left( T_{i-1,j,p}^{n+1} + T_{i+1,j,p}^{n+1} \right) \\
- Fo_y \left( T_{i,j-1,p}^{n+1} + T_{i,j+1,p}^{n+1} \right) - 2Fo_z T_{i,j,p-1}^{n+1} - 2Bi_zFo_z T_a - \frac{\partial t}{\rho c} q_{\text{node}},
\]

(3.10)

where \( q_{\text{node}} \) is the heat added to each node. \( q_{\text{node}} \) is obtained from the constant heat flux, \( q'' \) added to the top surface:

\[
d_{\text{node}} = \frac{q'' \partial x \partial y \partial z}{\partial x \partial y \partial z} = \frac{q''}{\partial z}.
\]

(3.11)

\( Bi_x, Bi_y, \) and \( Bi_z \) are the dimensionless Biot numbers defined in the \( x, y, \) and \( z \) directions for the discretized equations:

\[
Bi_x = \frac{h \partial x}{k},
\]

(3.12)

\[
Bi_y = \frac{h \partial y}{k},
\]

(3.13)

\[
Bi_z = \frac{h \partial z}{k}.
\]

(3.14)

Unheated boundary condition equation (Eq. (2.14)) results in five discretized equations which are applied to the nodes on: the unheated back surface, unheated front surface, unheated bottom surface, unheated bottom front line and unheated bottom back line. Equation (3.15) shows the discretized equation for unheated bottom back line:

\[
T_{i,l,1}^n = \left( 1 + 2Fo_x + 2Fo_y + 2Fo_z + 2Bi_zFo_z + 2Bi_yFo_y \right) T_{i,l,1}^{n+1} - Fo_x \left( T_{i-1,l,1}^{n+1} + T_{i+1,l,1}^{n+1} \right) \\
- 2Fo_y T_{i,l-1,1}^{n+1} - 2Fo_z T_{i,l,2}^{n+1} - 2Bi_zFo_z T_a - 2Bi_yFo_y T_a.
\]

(3.15)
Applying the Dirichlet boundary condition (Eq. (2.12)) creates 10 more discretized equations which impose the nodes at the left surface, and lines as well as the right surface and lines to be at the constant temperature $T_w$.

Table 3.1 summarizes the discretized equations for thermal analysis where $m$ is the number of nodes in the $x$ direction, $l$ is number of nodes in the $y$ direction, and $p$ is the number of nodes in the $z$ direction.

3.2.3.2. System of Equations (Matrix Construction and Solution). In order to solve the system of equations, one matrix and two vectors are defined: Coefficient matrix, KK, variable vector A, and constant vector B. Coefficient matrix KK is a $M$ by $M$ matrix which includes the coefficients multiplies in nodal temperature values at time $n+1$ ($T_{i,j,k}^{n+1}$) where $M$ is the total number of nodes in the domain. The coefficients are determined by the discretized equations shown in Table 3.1.

The vector A includes the unknown variables nodal temperature values at time $n+1$ ($T_{i,j,k}^{n+1}$). The vector B includes the constants including the constant wall temperature $T_w$ and nodal heat added to the nodes at the top boundaries. The nodes corresponding to no heat addition or convective boundary conditions, interior nodes, impose zero to the corresponding element in the matrix B. The system of equations should be set so $KK \times A = B$ satisfies the discretized equations.

Since the matrix KK and the vector B are constant, both of them are set outside of the transient loop (Figure. 3.2). The purpose is to obtain the vector A at each time step which includes the nodal temperature values at the next time step, $n+1$. An iterative Gauss Seidel method (Kreyszig, 2005) is used to solve the system of equations iteratively. When the iterative error reduces to the tolerance, the obtained nodal temperatures $T_{i,j,k}^{n+1}$ represent the temperature at the next time step. This means the previous nodal temperature values can be substituted with the current one to move to the next time step calculation.
Table 3.1. Thermal discretized equations

<table>
<thead>
<tr>
<th>Node location</th>
<th>Discretized Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left surface, and lines</td>
<td>$T_{1,j,k}^n = T_w$</td>
</tr>
<tr>
<td>Right surface, and lines</td>
<td>$T_{m,j,k}^n = T_w$</td>
</tr>
<tr>
<td>Interior nodes</td>
<td>$T_{i,j,k}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} \right] T_{i,j,k}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,j,k}^{n+1} + T_{i+1,j,k}^{n+1} \right) - F_{oy} \left( T_{i,j-1,k}^{n+1} + T_{i,j+1,k}^{n+1} \right) - F_{oz} \left( T_{i,j,k-1}^{n+1} + T_{i,j,k+1}^{n+1} \right)$</td>
</tr>
<tr>
<td>Top heated surface</td>
<td>$T_{i,j,p}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} + 2Bi_z F_{oz} \right] T_{i,j,p}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,j,p}^{n+1} + T_{i+1,j,p}^{n+1} \right) - F_{oy} \left( T_{i,j-1,p}^{n+1} + T_{i,j+1,p}^{n+1} \right) - 2F_{oz} T_{i,j,p}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- 2Bi_z F_{oz} T_a - \frac{\partial t}{\rho C} q_{node}$</td>
</tr>
<tr>
<td>Top front heated line</td>
<td>$T_{i,l,p}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} + 2Bi_z F_{oz} + 2Bi_y F_{oy} \right] T_{i,l,p}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,l,p}^{n+1} + T_{i+1,l,p}^{n+1} \right) - 2F_{oy} T_{i,2,p}^{n+1} - 2F_{oz} T_{i,l,p-1}^{n+1} - 2Bi_z F_{oz} T_a$</td>
</tr>
<tr>
<td></td>
<td>$- 2Bi_y F_{oz} T_a - \frac{\partial t}{\rho C} q_{node}$</td>
</tr>
<tr>
<td>Top back heated line</td>
<td>$T_{i,l,p}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} + 2Bi_z F_{oz} + 2Bi_y F_{oy} \right] T_{i,l,p}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,l,p}^{n+1} + T_{i+1,l,p}^{n+1} \right) - 2F_{oy} T_{i,j-1,p}^{n+1} - 2F_{oz} T_{i,l,p-1}^{n+1} - 2Bi_z F_{oz} T_a$</td>
</tr>
<tr>
<td></td>
<td>$- 2Bi_y F_{oz} T_a - \frac{\partial t}{\rho C} q_{node}$</td>
</tr>
<tr>
<td>Back unheated surface</td>
<td>$T_{i,l,k}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} + 2Bi_z F_{oz} + 2Bi_y F_{oy} \right] T_{i,l,k}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,j,k}^{n+1} + T_{i+1,j,k}^{n+1} \right) - F_{oz} \left( T_{i,j,k-1}^{n+1} + T_{i,j,k+1}^{n+1} \right) - 2F_{oy} T_{i,l,k}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- 2Bi_y F_{oz} T_a$</td>
</tr>
<tr>
<td>Front unheated surface</td>
<td>$T_{i,l,k}^n = \left[1 + 2F_{ox} + 2F_{oy} + 2F_{oz} + 2Bi_z F_{oz} + 2Bi_y F_{oy} \right] T_{i,l,k}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{ox} \left( T_{i-1,l,k}^{n+1} + T_{i+1,l,k}^{n+1} \right) - F_{oz} \left( T_{i,l,k-1}^{n+1} + T_{i,l,k+1}^{n+1} \right) - 2F_{oy} T_{i,l,k}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- 2Bi_y F_{oz} T_a$</td>
</tr>
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(Table 3.1. continued)

<table>
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<th>Discretized Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom unheated surface</td>
<td>$T_{i,j,1}^n = \left(1 + 2F_{o_x} + 2F_{o_y} + 2F_{o_z} + 2B_{i,y}F_{o_y}\right)T_{i,j,1}^{n+1}$</td>
</tr>
<tr>
<td></td>
<td>$- F_{o_x}\left(T_{i-1,j,1}^{n+1} + T_{i+1,j,1}^{n+1}\right) - F_{o_y}\left(T_{i,j-1,1}^{n+1} + T_{i,j+1,1}^{n+1}\right) - 2B_{i,y}F_{o_y}T_{a}$</td>
</tr>
<tr>
<td></td>
<td>$- 2B_{i,z}F_{o_z}T_{a}$</td>
</tr>
</tbody>
</table>

| Bottom front unheated line  | $T_{i,1,l}^n = \left(1 + 2F_{o_x} + 2F_{o_y} + 2F_{o_z} + 2B_{i,z}F_{o_z} + 2B_{i,y}F_{o_y}\right)T_{i,1,l}^{n+1}$ |
|                            | $- F_{o_x}\left(T_{i-1,1,l}^{n+1} + T_{i+1,1,l}^{n+1}\right) - 2F_{o_y}T_{i,2,1}^{n+1} - 2F_{o_z}T_{i,1,2}^{n+1} - 2B_{i,z}F_{o_z}T_{a}$ |
|                            | $- 2B_{i,y}F_{o_y}T_{a}$                                       |

| Bottom back unheated line   | $T_{i,l,1}^n = \left(1 + 2F_{o_x} + 2F_{o_y} + 2F_{o_z} + 2B_{i,z}F_{o_z} + 2B_{i,y}F_{o_y}\right)T_{i,l,1}^{n+1}$ |
|                            | $- F_{o_x}\left(T_{i-1,l,1}^{n+1} + T_{i+1,l,1}^{n+1}\right) - 2F_{o_y}T_{i,l-1,1}^{n+1} - 2F_{o_z}T_{i,l,2}^{n+1} - 2B_{i,z}F_{o_z}T_{a}$ |
|                            | $- 2B_{i,y}F_{o_y}T_{a}$                                       |

Structural equation, Eq. (2.34) is solved coupled with the thermal equations at each time step. The same approach as thermal analysis is used. The only difference is that this equation is one dimensional in the x direction. The integration for obtaining the thermal moment is performed using a trapezoidal method (Kreyszig, 2005). Next, the equation is discretized using the same central Finite Difference method used in thermal analysis. Since the beam is assumed pinned-pinned, zero displacement is imposed to both ends. The system of equations is constructed using one matrix and two vectors, and the system of equations is solved using a Gauss Seidel method.

Figure 3.2 shows the algorithm of the implemented code for solving thermal structural equation.
3.3 Non-dimensional Parameters

The results are non-dimensionalized using the Buckingham-Pi theorem (White, 2011). Eight physical variables are selected as $\delta$, $k$, $h$, $q''$, $L$, $W$, $d$, and $\alpha$. Here, $\delta$ is the center displacement which is the maximum displacement along the beam ($\delta=\nu(x=L/2)$). Four independent physical variables were selected as $\delta$, $k$, $l$, and $\alpha$. As a result, five dimensionless groups are obtained as follows:

$$\delta^* = \frac{\delta k}{q'' \alpha L^2},$$  \hfill (3.16)

$$Bi = \frac{h L}{k},$$  \hfill (3.17)

$$w^* = \frac{W}{L},$$  \hfill (3.18)

$$d^* = \frac{d}{L},$$  \hfill (3.19)
\[ \Delta T^* = \frac{\Delta T k}{q^* L}, \quad (3.20) \]

where \( \delta^* \) is the dimensionless center displacement. \( Bi \) is the Biot number. \( w^* \) and \( d^* \) are aspect ratios, \( \Delta T \) is the average temperature difference, and \( \Delta T^* \) is the dimensionless temperature difference. The dimensionless center displacement \( \delta^* \) is a function of dimensionless parameters \( Bi, w^* \), and \( d^* \).

### 3.4 Scaling of Statistical Effects

The displacement created by thermal stresses can be scaled against two nano-mechanical effects: quantum mechanical limits (Schwab and Roukes, 2005) and statistical mechanical effects (Stowe et al., 1997). Because quantum mechanical effects only appear in conduction and mechanical motion at low temperatures, they are ignored in this analysis. At room temperature, the statistical mechanics effects are measurable. The individual atoms of the cantilever are vibrating, causing a very small, but quantifiable displacement which is defined as thermal noise (Stowe et al., 1997; Datskos et al., 2003). In order to define the thermal noise, the mechanical stiffness \( k_s \) of the system is defined as (Young and Budynas, 2002):

\[ k_s = \frac{192EI}{L^3}. \quad (3.21) \]

The thermal displacement is calculated using the following formulation:

\[ \delta_{th} = \sqrt{\frac{k_b T}{k_s}}, \quad (3.22) \]

where \( T \) is the device temperature (Stowe et al., 1997).

The Displacement Ratio (DR) is defined as the center displacement, created by the thermal stresses, divided by the thermal displacement.

\[ DR = \frac{\delta}{\delta_{th}}. \quad (3.23) \]
The Displacement Ratio behavior will be a specific function of heat flux added to the top surface, \( q'' \). Dimensionless parameters are used to derive this function. The center displacement is a linear function of dimensionless center displacement \( (\delta-\delta^*) \). The thermal displacement changes with the square root of the temperature, as given in Eq. (3.22). The average temperature difference varies linearly by dimensionless temperature difference \( (\Delta T=(T-T_w)-\Delta T^*) \). Substituting Eq. (3.16) and (3.22) into Eq. (3.23), the Displacement Ratio is a function of \( q'' \), the geometry and material properties of the beam:

\[
DR = \frac{q'' \alpha L^2 \delta^*}{k \left( \frac{k_b}{k_s} \left( \frac{T_w + q''l\Delta T^*}{k} \right) \right)}, \tag{3.24}
\]

where \( \delta^* \) and \( \Delta T^* \) are functions of Biot number.

### 3.5 Results and Discussion

#### 3.5.1 Convergence and Validation

The model was run for \( 31 \times 9 \times 7 \) nodes in a quarter of the model. Grid independence was verified by repeating the simulations for \( 35 \times 13 \times 11 \), and \( 51 \times 25 \times 15 \). The results show that \( 35 \times 13 \times 11 \) is sufficient to obtain accurate results. Figure 3.3 shows the convergence history in linear (see a) and logarithmic (see b) scales. The temperature residuals decay to the convergence criteria which is \( 10^{-6} \).

Initial results for an unheated structure were compared with the analytical solution for a fin with a rectangular cross section (Incropera, 2007) to validate the discretization. The analytical solution for the temperature distribution along a fin with constant temperature \( T_w \) at both ends and ambient temperature of \( T_a \) is given in Eq (3.25):
\[ T(x) = (T_w - T_a) \frac{\sinh \left( \sqrt{\frac{2h(W + d)}{kWd}} x \right)}{\sinh \left( \sqrt{\frac{2h(W + d)}{kWd}} x \right)} + \sinh \left( \sqrt{\frac{2h(W + d)}{kWd}} (L - x) \right) + T_u. \]  

\hspace{1cm} (3.25)

Figure 3.3 Convergence history (a) Linear scale (b) Logarithmic scale

Figure 3.4 shows the analytical solution versus numerical solution for an unheated bridge with the wall temperature of 310 K and the ambient temperature of 290 K. The heat transfer coefficient is 411 W/m²K at the pressure of 100 Pa. The results are in good agreement for a bridge with a length of 100 microns.

Figure 3.4 Numerical results verified with analytical fin results
Figure 3.5 shows the displacement variations along the x axis for the free molecular model in silicon MEMS beam. The maximum displacement occurs at the center. This behavior agrees with the temperature distribution behavior, which shows displacement variations by total heat correspond to a linear system. This is qualitatively in agreement with experiments by Wang et al. (Wang, 2004). The simulation of nano-bridges shows a higher amount of heat is required to deflect the bridges in the order of angstroms.

![Graph showing displacement variations along the length of the bridge for different heat fluxes in MEMS beam](image)

**Figure. 3.5 Displacement variations along the length of the bridge for different heat fluxes in MEMS beam (Free molecular method - Bi=3.162e-6)**

### 3.5.2 Dimensional Results

Figure 3.6 (see a and b) show center displacement variations by pressure for silicon in the MEMS and NEMS beams. Figure 3.6 (see c and d) show the same variations for silicon carbide and CVD diamond in the NEMS beam. In all cases, the center displacement increases as the heat load increases. It is clear that center displacement is pressure-dependent in the free molecular approach due to the heat transfer coefficient, h. The heat transfer coefficient is pressure-dependent in the free molecular case as explained in section 2.4. In nano-scale models, center displacement behavior versus pressure was investigated for three different materials. The continuum and free molecular cases show a difference in center displacement of 10.5%, 13.5%, and 5.1% for silicon,
silicon carbide, and CVD diamond, respectively. The difference is less for CVD diamond because it is more conductive than the other materials. The percentage difference doubles in the micro-scale model. CVD diamond also shows center displacement of two orders of magnitude smaller than silicon and silicon carbide.

3.5.3 Non-dimensional Results

Figure 3.7 shows dimensionless temperature difference variations by the Biot number. The plots collapse for different materials. Equation (3.2) and (2.34) suggests that dimensionless center displacement $\delta^*$ can be obtained from $\Delta T^*$. This suggests that dimensionless center displacement plots versus Biot number are expected to collapse for different materials.
Figure 3.7 Dimensionless temperature difference versus the Biot number for different materials

Figure 3.8 shows the dimensionless center displacement of the bridge, versus the Biot number, for three different materials commonly used in micro-devices. The dimensionless center displacement plots collapse. It shows that the center displacement changes as a function of material properties, heat transfer coefficient, and the geometry. The results determine the power required to position the wave guide. This also gives an estimate of the power required to actuate the nanomechanical bridge used as a switch. The micro-scale silicon results also collapse with nano-scale results of other materials. It shows that as long as $w^*$ and $d^*$ are identical, the dimensionless center displacement will be identical. The results collapse for the micro- and nano-scales, which shows that the system behaves linearly.

Figure 3.8 Dimensionless displacement versus the Biot number for various materials
Figure 3.9 shows the changes of dimensionless center displacement of the bridge versus the Biot number in silicon, showing the effects of the geometry changes. As $L$ increases while $W$ and $d$ are constant, the displacement increases. These variations are more significant at high Biot numbers. These variations occur for two reasons. The heat flux added to the system by the heating laser or electrical heaters is constant. The first reason is that the total heat power at the top given in Eq. (3.26) increases due to the increase in the top surface area:

$$q = q^* L W.$$  \hfill (3.26)

The second reason is that the displacement varies relatively with the length of the bridge. The study of width variations effects on the dimensionless center displacement is performed. The length $L$ and thickness $d$ remain constant while only width $W$ of the bridge decreases. The displacement decreases due to the decrease in the total laser heat power, but the displacement variation is negligible. Also, the bridge thickness variation effect on the displacement is investigated at constant $L$ and $W$. Any decrease in the thickness results in an increase in the displacement due to the volume reduction for the same total heat though the variations are negligible.

![Figure 3.9 Dimensionless displacement versus the Biot number: (a) For different materials, (b) For different bridge lengths](image)
3.5.4 Statistical Effects

Figure 3.10 shows the thermal displacement variations by temperature for silicon, silicon carbide and CVD diamond in nano scale, and silicon in micro scale (Eq. (3.22)). The thermal noise of silicon carbide and CVD diamond is in the order of tens of angstroms. This value is much larger for silicon due to its smaller modulus of elasticity. This suggests silicon carbide or CVD diamond may be the preferred material for these systems. Because of the increased stiffness, the micro-scale silicon device generates less noise in comparison with nano-devices.

As shown in Figure 3.10, CVD diamond shows the least thermal noise while silicon shows the largest. However, Figure 3.6 (see d) shows the center displacements in a CVD diamond nano-device are so small that an increase in the heat load will not make the results to be physically meaningful. In contrast, Figure 3.6 (see b) shows that a significant increase in the heat load might overcome the noise problem for silicon.

Figure 3.10 Thermal displacement versus temperature variations

Figure 3.11 shows Displacement Ratio variations by heat flux added to the top surface, for three different materials in nano-scale. Heat transfer coefficient is calculated based on free molecular approach at 0.1 Pa. The largest DR belongs to silicon carbide. As shown in Figure 3.10, silicon carbide has relatively low thermal displacement due to its large modulus of elasticity while
it has the highest center displacement among all materials as shown in Figure 3.6 (see c). Since temperature increase variations by heat flux corresponds to a linear system, Eq. (3.24) shows that Displacement Ratio increases by the square root of the temperature increase.

![Figure 3.11 Displacement Ratio (DR) for three different materials at P_{air}=0.1 \text{ Pa}](image1)

Figure 3.11 Displacement Ratio (DR) for three different materials at P_{air}=0.1 \text{ Pa}

Figure 3.12 shows Displacement Ratio variations by heat flux, for silicon carbide at two different Biot numbers. As the heat flux increases the Biot number has a noticeable effect on the Displacement Ratio.

![Figure 3.12 Displacement Ratio (DR) (Silicon carbide-Free Molecular)](image2)

Figure 3.12 Displacement Ratio (DR) (Silicon carbide-Free Molecular)

3.6 Conclusion

The implicit Finite Difference method is more suitable than the explicit one due to unconditional stability. Simulations are performed by coupling thermo-structural equations at each time step. The simulation results draw the following conclusions:
(1) Ambient cooling strongly influences the displacement of thermally-positioned nano-scale devices. The Biot number determines the dimensionless displacement of the bridge.

(2) The displacement of the system is a function of the geometry. The results show that as the ratio of the width to the length of the bridge decreases for constant widths, the value of displacement increases.

(3) The displacement behavior is also a function of pressure, material properties, and constant heat flux in free molecular model, while this value is independent of pressure in the continuum model. The displacement increases as the constant heat flux at the top surface increases. This behavior shows that the displacement variations by total heat added to the structure in this model corresponds to that of a linear system.

(4) As the dimensions of a geometry change by a constant factor, the dimensionless displacement versus the Biot number collapse in all cases for the same material property.

(5) Thermal noise analysis and the displacement variations by pressure suggest silicon carbide as the most appropriate material to fabricate nano-devices where positioning accuracy is a design requirement. It shows the displacements of the order of angstrom for an average heat load and thermal noises of tens of the order of the magnitude.
CHAPTER 4: THERMALLY ACTUATED MICRO-SWITCHES: AN APPLICATION TO STEADY RESPONSE TO CONSTANT HEATING

In 2001, Blondy et al. fabricated a thermally actuated silicon nitride micro-switch bridge. The heat was added to the sides of the top surface of the switch. Their experimental measurements showed that the switch had low actuation voltage. The switch also offered high isolation, and mechanical protection (Blondy et al., 2001). This chapter analyses the power usage and optimization of the switch designed by Blondy et al. (Maghsoudi and Martin, 2012b).

Three heating configurations are used: distributed heat at the top surface, concentrated heat at the center of the top surface, and concentrated heat at the sides of the top surface. The study of various heating configurations gives the opportunity to compare the alternative heating configurations for Blondy’s design and increase the efficiency.

At time t=0, a constant heat load, q, ranging from 1.4 W to 6.25 W, is applied to the top of the bridge until the bridge reaches a thermally steady state condition. The heating procedure is also performed for closed-switch models with different thermal boundary conditions. Simulations are performed for two different materials: silicon and silicon nitride.

4.1 Geometry and Boundary Conditions

The geometry is a 3-dimensional pinned-pinned beam as shown in Figure 3.1 in Chapter 3, with a length L of 250 microns, a width W of 50 microns, and a thickness d of 1 micron. Conduction within the beam as well as convection between the beam and the quiescent gas are considered. Hence, there is convection of heat from the wall to the gas and conduction of heat through the bridge to the wall. The heat losses through the contact are considered when the bridge is closed. The thin film resistor heat addition is modeled as a constant heat load, q”, applied to the top surface of the beam. This also corresponds to the heat addition of a thin resistive film.
4.1 (see a and b) show the geometry and boundary conditions for distributed heat addition. Figure 4.1 shows the open-switch model (see a) and the close-switch model (see b).

![Diagram](image)

(a)

Figure. 4.1 The geometry and boundary conditions (a) Distributed heat in open switch (b) Distributed heat in closed switch

There are two alternative heating configurations shown in Figure 4.2. Figure 4.2 shows the geometry and boundary conditions for center-heating configuration (see a) and shows the geometry and boundary conditions for side-heating configuration (see b).

![Diagram](image)

(a)

Figure. 4.2 The geometry and boundary conditions for open switch with (a) Concentrated heat at the top center (b) Concentrated heat at the sides of the top surface
4.2 Formulation and Simulation Method

Simulation of thermal actuation of micro-devices, and the computation of the mechanical response of the system, in this case the displacement, requires a thermo-structural formulation for this problem. The same thermo-structural formulation including governing equations, and boundary conditions which are defined in chapter 3 (section 3.2) is applied to this problem. The free molecular heat transfer coefficient, $h$ is defined as Eq. (2.17):

$$h = \sigma_T n_i \frac{\gamma + 1}{\gamma - 1} \sqrt{\frac{k_b T_a}{8\pi m}},$$

where $\sigma_T$ is the thermal accommodation coefficient, $\gamma$ is the specific heat ratio of the gas, $m$ is the molecular weight of the gas, and $n_i$ is the number density of the gas. For an ideal gas, $n_i$ can be calculated using

$$n_i = \frac{P_{\text{gas}}}{m RT_a},$$

where $R$ is the ideal gas constant.

The 3-dimensional transient heat conduction equation is the thermal governing equation of the model:

$$\frac{\partial T(x,y,z,t)}{\partial t} = \frac{k}{\rho c_p} \left( \frac{\partial^2 T(x,y,z,t)}{\partial x^2} + \frac{\partial^2 T(x,y,z,t)}{\partial y^2} + \frac{\partial^2 T(x,y,z,t)}{\partial z^2} \right),$$

where $k$ is the thermal conductivity, $\rho$ is the density, and $c_p$ is the specific heat of the solid. $T$ is the temperature distribution in the solid.

4.2.1 Open Switch Simulation

The thermal governing equation for both the open and closed-switch models is the same. Equation (2.1) is used to obtain the temperature distribution at each time step in the model.
However, the thermal boundary conditions are different for open and closed switch models as shown in Figure 4.1.

There are three different types of boundary conditions in the open-switch model as shown in Figure 4.1 (see a) and 4.2 (see a and b). The Dirichlet boundary condition as shown in Eq. (2.12) is applied to the ends of the bridge when the switch is open.

\[ T = T_w. \]  

(2.12)

There are two different types of Neumann boundary conditions which are applied to heated and unheated surfaces. Equation (2.13) shows the boundary condition for the top heated surface, and Eq. (2.14) shows the boundary condition for unheated surfaces.

\[ -k \frac{\partial T}{\partial n} = h(T - T_a) + q'', \]  

(2.13)

\[ -k \frac{\partial T}{\partial n} = h(T - T_w). \]  

(2.14)

Equation (2.14) is applied to the entire top surface for distributed heating configuration as shown in Figure 4.1 (see a). However, it is only applied to the heated surfaces at the top for the center heating and side heating configurations as shown in Figure 4.2 (see a and b).

At time \( t=0 \) a calculated heat flux corresponding to a constant heat, \( q \) is added to the system. In each time step, the heat conduction equation (Eq. (2.1)) along with open-switch boundary conditions (Eqs. (2.12) to (2.14)) is solved numerically using a finite difference method. The solution gives the nodal temperature distribution in the bridge.

Using the nodal temperature values, the thermal moment due to thermal stresses as previously shown in Eq. (3.2) is obtained:

\[ M_{th}(x,t) = E \int \alpha(T - T_w)z dA. \]  

(3.2)
In order to obtain the displacement distribution along the beam, Eq. (2.34) is numerically solved using a Finite Difference method:

\[ EI \frac{\partial^2 \nu(x,t)}{\partial x^2} + M_m = 0. \]  

(2.34)

The moment and displacement are zero at both ends for pinned-pinned boundary condition:

\[ \nu(x = 0, L) = 0. \]  

(2.35)

Calculations of the nodal temperature values and displacement distribution at each time step continue until the system reaches thermal steady state. The corresponding center displacement at this point is called the thermally steady state center displacement, \( \delta_T \).

The closing displacement, \( \delta_c \) is defined as a sufficiently large displacement to touch the contact surface at the closing time. In order to obtain the closing displacement, the dynamic structural equation must be simulated. The dynamic structural equation is not solved in this work. Instead, the steady state structural equation is simulated to obtain thermally steady state center displacement. The thermally steady state center displacement, \( \delta_T \) is not necessarily the closing displacement, \( \delta_c \) at which the switch is assumed closed. It can be larger or smaller depending on the value of the heat added to the system. The overall efficiency coefficient of the switch will be the displacement per power added. This can be defined as \( \eta^* \):

\[ \eta^* = \frac{\delta_T}{q} = \frac{\delta_T}{q^* \cdot L \cdot W}, \]  

(4.1)

where \( q \) is the total rate at which heat is added to the switch.

### 4.2.2 Closed Switch Simulation

When the switch touches the contact a reaction displacement \( \delta_R \) is created due to a reaction force. This means it is necessary to continue heating the device to keep the switch closed. As heat addition to the system continues by time after the switch is closed, the value of reaction force
increases, leading to the increase in the reaction displacement. In this case, $\delta_T$ increases to compensate the increase in $\delta_R$ in the opposite direction and keep the switch closed. The reaction displacement relates with $\delta_T$ and $\delta_c$ as:

$$\delta_R = \delta_c - \delta_T.$$  \hfill (4.2)

In order to study the required heat to keep the switch closed, thermal boundary conditions are changed to closed-switch model’s thermal boundary conditions as shown in Figure 4.1 (see b). Dirichlet boundary condition shown in Eq. (2.12) is applied to the contact as well as the both ends. The study begins with the contact temperature $T_c$ equal to the wall temperature. In section 4.4 the study continues for various contact temperatures. Neumann boundary conditions remain unchanged as shown in Eqs. (2.13) and (2.14). The procedure explained in section 4.2.1 is performed to obtain the thermal steady state displacement, $\delta_T$.

4.3 Results and Discussion

The analytical solution of a fin with rectangular cross section validates the results for the boundary conditions without the added heat flux. The model is run for $31 \times 9 \times 7$ nodes in a quarter of the model. Grid independence is verified by repeating the simulations for $35 \times 13 \times 11$, and $51 \times 25 \times 15$. The results show that $35 \times 13 \times 11$ is sufficient to obtain accurate results.

4.3.1 Materials

The material study begins with silicon which is a standard material for nano- and micro-fabrication. It continues with the most common material for thermal switches, silicon nitride (Blondy et al., 2001). Other materials used for micro-switches, such as Ti/gold and quartz, are not appropriate for thermal actuation applications (Rebeiz, 2003).
Simulations are performed for two different materials: silicon and silicon nitride. The thermal properties of materials are assumed to be constant and defined at wall temperature as shown in Table 4.1.

Figure 4.3 shows thermal steady state displacement variations by heating rate for silicon and silicon nitride. The steady state results show that the thermal steady state displacement variation at the center of the bridge versus the total heat changes at the top corresponds to a linear system. Furthermore, for a constant heating rate, silicon nitride shows overall efficiency coefficient $\eta^*$ of 5.6 times larger than silicon’s $\eta^*$. Silicon nitride is selected for the rest of the study.

<table>
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<th>$c_p$ (J/kg.K)</th>
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<th>$\alpha$ ($10^{-6}$×1/K)</th>
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</tr>
<tr>
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<td>300</td>
</tr>
</tbody>
</table>

Figure 4.3 Thermal steady state displacement versus heating rate for silicon and silicon nitride

### 4.3.2 Open versus Closed Model

Steady state results are obtained to compare the open switch behavior with the closed switch. Figure 4.4 shows the thermal steady state displacement variations with the heating rate for silicon nitride open-switch and closed-switch models. For a specific $\delta_T$ at the center, the closed bridge
requires less heating rate than the free bridge. The open silicon nitride bridge shows $\eta^*$ of 66.1 nm/W, while the closed silicon nitride bridge shows $\eta^*$ of 89.1 nm/W.

These results show that the closed bridge requires less power to remain in closed position than the power the open bridge requires reach the closed position. This means that the switch is effectively over-powered when in the closed position. Even if the heaters are sized perfectly to close the bridge, there will be excess heating in the closed configuration. When power is removed, the switch will not open immediately. The switch will have to cool down by this extra amount before it can open.

**4.3.3 Heating Configurations Efficiency**

In order to optimize the heat addition, two additional heating configurations are studied. The first approach is to add concentrated heat at the center of the top surface, which will be referred to the center-heating configuration. Current switches add heat at the base of the bridge, which will be referred to as the side-heating configuration (Blondy et al., 2001). The approach of adding heat uniformly along the top of the bridge will be referred to the distributed-heating configuration. Each of these configurations corresponds to a different placement of the heaters used in thermal actuation.
Figures 4.5 shows the steady state results for new models and distributed-heating for open (see a) and closed (see b) switches. The center-heating configuration shows the largest thermal steady state displacement among all models for the same total heat added to the top. Table 4.2 summarized overall efficiency coefficient, $\eta^*$ for the contact length of 14 microns and the heating length of 40 microns for the side and center-heating configurations.

<table>
<thead>
<tr>
<th>Heating Configuration</th>
<th>Open Switch $\eta^*$ (nm/W)</th>
<th>Closed Switch $\eta^*$ (nm/W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distributed</td>
<td>66.1</td>
<td>89.1</td>
</tr>
<tr>
<td>Center</td>
<td>101.25</td>
<td>201.5</td>
</tr>
<tr>
<td>Side</td>
<td>11.5</td>
<td>11.4</td>
</tr>
</tbody>
</table>

The center-heating configuration shows the overall efficiency coefficient $\eta^*$ of 101.25 nm/W for open-switch. This value decreases to 66.1 nm/W for distributed-heating and 11.5 nm/W for side-heating open-switch as shown in Table 4.2. It shows the center-heating configuration is 8.8 times and distributed-heating configuration is 5.7 times more efficient than the side-heating configuration.
As previously discussed, a closed switch shows larger overall efficiency coefficient than an open switch for distributed heat configuration. The overall efficiency coefficient changes from 66.1 nm/W in open switch to 89.1 nm/W in closed switch.

The center-heating configuration follows the same behavior while the side-heating configuration does not. Center-heating the closed switch increases the overall efficiency coefficient from 101.25 nm/W to 201.5 nm/W. However, this value decreases from 11.5 nm/W to 11.4 nm/W for side-heating the closed-switch. Study of the temperature distribution in x-z plane clarifies the reason. The temperature gradient along the z axis determines the magnitude of the displacement as shown in Eq (4.3):

\[
\frac{d^2 \nu(x)}{dx^2} = \frac{\alpha}{I} \int_{\text{Area}} (T_a - T(x, y, z)) \, dy \, dz,
\]

where Eq. (4.3) is obtained using Eq. (3.2) and (2.34).

Figure 4.6 shows the mid plane cross section along the x axis. Temperature distributions for various heating configurations illustrated in Figures 4.7 to 4.9 are plotted in this mid plane. The temperature distribution is plotted as temperature difference, T-T_w.

![Diagram of mid-plane cross section along the x axis](image)

Figure. 4.6 Mid-plane cross section along the x axis

Figure 4.8 shows the temperature distribution in mid plane for center heating configuration for open-switch (see a) and closed-switch (see b) model. When the heat is added to the center, wall temperature boundary condition at the contact in closed bridge enhances the temperature gradient
in the $z$ direction. The increase in temperature gradient along the $z$ axis leads to an increase in the thermal steady state displacement. As a result overall efficiency coefficient increases (Eq. (4.1)). The same behavior is observed for distributed-heating configuration as shown in Figure 4.7.

Figure 4.7 Temperature distribution in the mid plane (a) distributed heating configuration open-switch model (b) distributed heating configuration closed-switch model

Figure 4.8 Temperature distribution in the mid plane (a) Center-heating configuration open-switch model (b) Center-heating configuration closed-switch model
However, this phenomenon does not occur for the side-heating configuration. In this case, the switch is more efficient when open. This means the switch may reach the closed position, lose heat, and re-open. This can only be avoided by over-sizing the heaters.

Figures 4.9 shows the temperature distribution in mid plane for side-heating configuration for open-switch (see a) and closed-switch (see b) models, respectively. When the switch is closed, wall temperature boundary condition at the contact does not enhance the temperature gradient in the z direction (Figure. 4.9 (see b)). It means more energy is required to keep the switch closed when side-heating configuration is used.

![Figure 4.9 Temperature distribution in the mid plane (a) Side-heating configuration open-switch model (b) Side-heating configuration closed-switch model](image)

In center-heating and side-heating configurations the switch efficiency coefficient is a function of heating length. As long as the heating length affects the temperature gradient in the z direction, it can change the efficiency coefficient. Figure 4.10 shows the efficiency coefficient variations for center-heating and side-heating configurations and both open and closed switch. The efficiency variation is studied with the heating length from 20 microns to 120 microns in both cases.
Figure 4.10 Efficiency coefficient variation by the heating length

For the center-heating configuration, the efficiency increases as the heating length, $L_h$ increases up to 50 microns. Any increase in the heating length over 50 microns leads to a decrease in the switch efficiency. For both open and closed switches, 50 microns returns the maximum pick of the efficiency coefficient in center-heating configuration. The efficiency decays by increasing the heating length further than 120 microns and eventually it becomes equal to the efficiency coefficient of distributed heat configuration.

The side heating configuration’s efficiency coefficient increases linearly by the heating length. The efficiency difference between the open and closed switch is ignorable for the heating length up to 120 micron. The efficiency is expected to merge with the distributed heat’s efficiency coefficient as the heating length increases up to 250 microns.

4.3.4 Contact Effects

In order to study the effect of the contact length $L_c$ on the efficiency coefficient, contact lengths of 7, 14 and 21 microns are selected. The results show the maximum difference of less than 3 nanometers in the steady state center displacement. Table 4.3 shows the $\delta_T$ and $\eta^*$ variations by increasing the contact length. The thermal steady state center displacement increases from 54.15 nm to 55.7 nm when the contact length increases from 7 to 14 microns. It has 4% decrease in the
switch thermal efficiency. The efficiency coefficient and steady state thermal displacement remain constant as the contact length increases to 21 microns.

Table 4.3 Contact length effects on the efficiency for distributed heat (625 mW-SiN)

<table>
<thead>
<tr>
<th>L_c (µm)</th>
<th>7</th>
<th>14</th>
<th>21</th>
</tr>
</thead>
<tbody>
<tr>
<td>δT (nm)</td>
<td>54.15</td>
<td>55.71</td>
<td>55.71</td>
</tr>
<tr>
<td>η* (nm/W)</td>
<td>85</td>
<td>89.1</td>
<td>89.1</td>
</tr>
</tbody>
</table>

Increase of contact length further than 14 microns only affects the temperature gradient in the x direction which does not affect the thermal steady state center displacement.

Another parameter may affect the switch efficiency is the contact temperature T_c. The results presented in Figures 4.3 to 4.10 are obtained for the contact temperature T_c equal to the wall temperature T_w. The thermal conductance for a 0.12 microns gold contact is given as 0.1 mW/K which is a small value. A temperature increase of 20 to 30 C in the contact is enough to soften the contact area and lower the hardness of the contact material (Rebeiz, 2003). As a result, the temperature increase in the contact must not exceed 15 C. The contact temperature study is performed for T_c of 290, 295, 300 and 305 K. The contact temperature increase will decrease the temperature gradient in the z direction leading to the lower efficiency. Figure 4.11 shows the temperature difference distribution in the mid-plane for contact temperature of 295 K (see a) and 305 K (see b). The lower temperature gradient is observed in T_c of 305 K. However, the efficiency decrease is 1.5% for contact temperature increase from 290 K to 305 K.
4.4 Conclusion

The following conclusions can be drawn from these results:

Steady state results for distributed heat configuration and center-heating configuration show the closed switch operates more efficiently than open switch. This will lead to a thermal lag in opening the switch.

For a specific steady state center displacement for distributed heat configuration, closed switch requires less heat at the top than open switch. Open silicon-nitride-bridge shows the overall efficiency coefficient of 66.1 nm/W while closed silicon-nitride-bridge shows the overall efficiency coefficient of 89.1 nm/W.

Both the contact length and contact temperature variations have negligible effects on the steady state center displacement of the bridge. The contact length decreases to half results in the maximum difference of less than 3 nanometer in the steady state center displacement.

Heat addition to the center of the top surface of the bridge is the most efficient way to obtain a larger center displacement per unit heat addition. It is more thermally efficient than adding concentrated heat to the sides of the top surface by a factor of 17 in closed switch and 8.8 in open switch.
The qualitative difference in switch behavior in the open and closed positions will have implications for switch design. Switches that were side-heated became less efficient when closed, requiring additional heat to remain closed. In micro-device design, this effect has led to thermal-ratcheting approaches to prevent the switch from re-opening. These results suggest that this effect can be mitigated through heater design, offering a mechanically simpler alternative.
CHAPTER 5: TRANSIENT RESPONSE TO CONSTANT HEATING WITH APPLICATIONS TO NANO-MECHANICAL MEMORY

This chapter applies the two technologies of buckling beam and thermal excitation to design a storage memory. A unit bridge of an array of buckling-beam memory (a thermally actuated nano-bridge) is simulated using a Finite Difference method. Power requirements for thermal actuations, optimal geometry, and write time of the device for various materials are investigated. This type of storage memory can be applied to high radiation environments encountered in space exploration. The suggested memory is radiation protected against high energy particle collisions in high radiation environments such as Europa, moon of Jupiter.

5.1 Spacecraft Storage Memory Requirements

The design of computer systems for spacecraft is complicated by three constraints beyond those found in terrestrial systems: limited available power, a harsh environment, and the need for increased reliability (Griffin and French, 2004). The power constraint is the most severe for missions designed to go beyond the reach of available solar power, including missions to asteroids and exploration of Saturn and Jupiter’s moons. Several of these missions, especially exploration of Io and Europa, are likely future targets for NASA missions (Committee on the planetary science decadal survey, 2011).

The environmental constraints include extremes of temperature far beyond those encountered by terrestrial electronics, high radiation levels, and, in some cases, strong magnetic fields. The critical role spacecraft electronics play in mission navigation, and in returning scientific data to earth, requires them to reach standards of reliability beyond those of any terrestrial systems. Spacecraft memory is affected by all of these constraints. The radiation constraint is the most difficult for these systems, and is the largest barrier to qualification of memory systems for
In the highly radioactive environment of space, high energy protons and electrons may strike the structure. These particles can be a result of solar events or the planetary environment (Fortescue et al., 2003). This can cause the single event upset for conventional semi-conductor devices. Current missions to the Jovian system use a radiation locker for all the electronics to avoid scrambling the data in conventional memories. In spite of this, the life of the current Juno mission is expected to be limited by radiation damage. NASA has recognized the need for new nano-technology based electronic systems for the future missions (Meador et al., 2010). This has led to the consideration of exotic memory systems for spacecraft applications, such as nano-tube based switches (Rueckes et al., 2000).

Improving the performance of the memory is one of the significant steps in the design of a memory system. The high performance memories require a high memory density, less power consumption, and fast write/read and erase times. At the present time, there is no memory designed to satisfy all mentioned performance aspects. For example, Phase Change random access Memories (PCM) have very low power consumption. The reported required energy for writing and reading data is in the order of 0.1 and 10 nJ respectively (Zhou et al., 2009). However, PCM do not write, read and erase as fast as Dynamic Random Access Memories (DRAM) (Philip Wong et al., 2010). Another example is molecular memories which have memory densities as high as $10^{12}$ bits/cm$^2$ (Chung et al., 2010; Paydavosi et al., 2011). In the design of memories for spacecraft, reliability requirements increase, due to the long service life of the systems, the inability to repair the system, and the mission-critical role of spacecraft electronics. An additional challenge is functioning in high radiation environments where high energy particle collisions can scramble the data.

The performance of a memory system strongly depends on its operational system. Most of the recent memories such as volatile or non-volatile nano-crystal memories (Steimle et al., 2003; De
Blauwe, 2002) and magnetoresistive random access memories (Engel et al., 2002) operate purely electrostatically. The concept of mechanical bistability of a doubly clamped bridge was used to implement non-volatile electro-mechanical memory (Nagami et al., 2010) and volatile mechanical memory (Badzey et al., 2004) operating based on the displacement of the bridge. A potentially simpler non-volatile memory device is the buckled-beam nano-mechanical memory (Hälg et al., 1990; Roodenburg et al., 2009; Charlot et al., 2008). These devices have been electrostatically actuated. After the beam is buckled through application of an electrostatically generated force, the bistable beam remains buckled after the power is removed. These devices have been successfully demonstrated in laboratory experiments (Roodenburg et al., 2009), but have not been the subject of extensive performance or reliability analysis.

5.2 Theory

Buckling of the beam is one of the essential concepts in the design of the suggested memory. In this section, the theory of buckling and bistable beams including single materials and membranes are briefly explained. Then, the operation of the memory device is discussed.

5.2.1 Theory of Buckling (Beer et al., 2001)

The stability of the structure is defined as its ability to support a given load without experiencing a sudden change in its configuration. Figure 5.1 shows two rigid rods connected by a pin and a torsional spring of constant $k_{sp}$.

![Figure 5.1 Stability in two rigid rods and spring system (Beer et al., 2001)](image-url)
As shown in Figure 5.1 (see a) the system is stable at the beginning while the connection pin is slightly moved to the right eventually (see b). In this case, there are two forces acting on the beam: the couple formed by P and P’, of moment $P(L/2)\sin(\Delta \theta)$, which tends to move the rod away from the vertical, and the couple $M_{sp}$ exerted by the spring, which tends to bring the rod back into its original vertical position. Assuming the angle of deflection of the spring is $2\Delta \theta$, the moment of the couple $M_{sp}$ is

$$M_{sp} = K_{sp}(2\Delta \theta). \quad (5.1)$$

If $M_{sp}$ is larger than the couple formed by P and P’, the system tends to return to its original equilibrium position as shown in Figure 5.1 (see a). In this case, the system is called stable. However, if the moment of the couple formed by P and P’ is larger than $M_{sp}$ the system tends to move away from its original equilibrium position and is called unstable. The critical load $P_{cr}$ is the value of the load for which the two couples balance each other as shown in Eq. (5.2).

$$P_{cr} \frac{L}{2} \sin(\Delta \theta) = K_{sp}(2\Delta \theta). \quad (5.2)$$

For a small angle $\Delta \theta$, $\sin(\Delta \theta) \approx \Delta \theta$,

$$P_{cr} = \frac{4K_{sp}}{L}. \quad (5.3)$$

In summary, the system is stable for $P<P_{cr}$ and unstable for $P>P_{cr}$.

Suppose designing a column of length L to support a given load P as shown in Figure 5.2 (see a). In this example, the column is pin-connected at both ends and the load P is a centric axial load. If $P>P_{cr}$ the slightest misalignment or disturbance buckles the column to a curved shape (see b).
Using the equilibrium of the free body AQ shown in Figure 5.3, the linear, homogeneous differential equation of the second order with constant coefficient is obtained as follows:

\[
\frac{d^2y}{dx^2} + \frac{P}{EI} y = 0. \quad (5.4)
\]

The general solution of Eq. (5.4) is

\[
y = A \sin(\sqrt{\frac{P}{EI}} x) + B \cos(\sqrt{\frac{P}{EI}} x). \quad (5.5)
\]

The boundary condition \(x=0, y=0\) gives \(B=0\) in Eq. (5.5). Substituting the second boundary condition \(x=L, y=0\) will give

\[
A \sin(\sqrt{\frac{P}{EI}} L) = 0. \quad (5.6)
\]
Equation (5.6) is satisfied either if $A=0$, or if the sin term is zero. If $A=0$, Eq. (5.5) reduces to $y=0$ representing the straight column shown in Figure 5.2 (see a). For the second condition to be satisfied, the following equation imposes the sin term to be zero:

$$\sqrt{\frac{P}{EI}}L = n\pi,$$

which gives the following for $P$:

$$P = EI\left(\frac{n\pi}{L}\right)^2.$$  \hfill (5.7)

The smallest of the values of $P$ defined by Eq. (5.8) is that corresponding to $n=1$. Substituting $n=1$ in Eq. (5.8), the critical load is given as follows for a pinned-pinned column:

$$P_{cr} = EI\left(\frac{\pi}{L}\right)^2.$$  \hfill (5.9)

Equation (5.9) gives the critical load only for a pinned-pinned beam. The general form of the critical buckling load is given as follows:

$$P_{cr} = EI\left(\frac{\pi}{L_e}\right)^2,$$  \hfill (5.10)

where $L_e$ is the effective length column depending on the boundary conditions applied to Eqs. (5.4) and (5.5). Figure 5.4 shows the effective length column for four different column boundary conditions. In this study, the critical buckling load corresponding to fixed-fixed boundary conditions is used as shown in Figure 5.4 (see d).
5.2.2 Bistable Buckling Beams

A thin, buckled, micromechanical bridge has been reported with two stable mechanical states, which could be switched up and down by electrostatic forces (Halg, 1990 and Roodenburg et. al., 2009). Figure 5.5 shows the schematic of the buckling beam. The buckling beam is highly compressed, so that the free standing part of it is stress-relieved, buckles and become mechanically bistable. As shown in Eq. (5.10), lower modulus of elasticity provides a smaller critical buckling force. In order to make the beam bistable, the buckling behavior must remain within the elastic regime. SiO$_2$ was used due to its low modulus of elasticity, E and the large elastic range (Halg, 1990). The transition between two buckling states was performed by electrostatic actuation. The electrostatic forces are created by application of a voltage between the bridge and an adjacent electrode. The substrate was used as an electrode to pull the bridge downward. The lateral electrodes where used to switch the bridge to the other stable state. A thin layer of Cr was sputtered on the top of the bridge to provide a conductive path to make the switching by electrostatic forces possible (Halg, 1990). In a similar design, a 600 nm layer of aluminum was used at the top of the bridge (Roodenburg et. al.).
The experimental analysis were performed for a range of buckling beams with the lengths of 10, 14, 20 and 40 microns. The microphotographs of the experiments showed that the bridge is in the mechanically stable “up” and “down” states as shown in Figure 5.6. The previous studies on bistable buckling beams showed that these structures are reliable over thousands of switching the buckling state cycles (Halg, 1990 and Roodenburg et. al., 2009).

It is reported that for the single material buckling beam samples with a small switching voltage (40 ±10 V) the bridges tend to become monostable. For example, they always relax in the “up” state. The possible reason is a tensile built-in stress in the metal layer on the top of the bridge which induces a large stress gradient across the thickness of the bridge leading to a considerable bending moment. As a results using a sandwich structure is strongly suggested (Halg, 1990).
Sandwich structures such as membranes were fabricated and tested as bistable buckling beams. Figure 5.7 shows a cross-sectional diagram of a snapping membrane structure (Arya et al., 2006). The device consists of a thin silicon (Si) membrane fixed at both ends with a layer of thermally grown silicon dioxide (SiO$_2$) with a comparable thickness at the top. In the first step, the temperature increases up to the oxidizing temperature (1000°C) at which the oxide flows plastically, leaving the silicon free of mechanical stresses.

After the silicon is cooled, the oxide layer hardens into an elastic material with a low coefficient of thermal expansion ($0.5 \times 10^{-6}$ K$^{-1}$) which is much smaller than that of silicon ($2.3 \times 10^{-6}$ K$^{-1}$). Cooling to the room temperature induces large stresses at the silicon/oxide interface. The stress state is biaxial compression in the oxide and biaxial tension in the underlying silicon. This system of stress will cause the membrane to buckle upward towards the oxide layer. The upward buckled configuration is stable and the deflected shape remains unchanged in the absence of any external mechanical force. However, a second stable state of mechanical equilibrium exists. If sufficient force is applied in the downward direction to the center of the membrane, the membrane buckles downward. The buckled downward shape is stable against small mechanical perturbations. A nearly flat equilibrium state which is approximately midway between the upward- and downward buckled states, is mechanically unstable. As a result, this system is called bistable.

The transition from the upward stable state to the downward stable state occurs using different methods. In Arya’s design it occurs by an increase in the ambient temperature. A layer of aluminum is deposited underside of the membrane as shown in Figure 5.7 when it is in the upward-
buckled state. The aluminum coefficient of thermal expansion ($23 \times 10^{-6} \text{ K}^{-1}$) is ten times that of silicon. When the membrane is heated, the aluminum layer attempts to expand at a much faster rate than the silicon and oxide layers. When a sufficient high temperature has been reached, a biaxial state of compression is induced in the aluminum counteracting the effect of the compression in the oxide layer and disappears the upward-buckled stable equilibrium state. As a result, the membrane snaps downward, into the single remaining stable state. The upward- and downward-buckled states exist in a range of temperatures that includes room temperature.

Matoba reported a similar bistable membrane design as shown in Figure 5.8 (Matoba et al., 1994). The U-shaped bistable cantilever membrane consists of three thin-film layered materials: polycrystalline silicon, silicon dioxide and polycrystalline silicon. The tension band is made of silicon nitride. This design uses resistive dissipation to heat the upper and lower layers of the cantilever for the transition from one stable state to another.

![Figure 5.8 Schematic view to demonstrate the transition between two stable states (Matoba et al., 1994)](image_url)

**5.2.3 Buckling Beam Memory**

Figure 5.9 illustrates the suggested buckling-beam memory system which uses an array of nanofabricated beams and thermal buckling of these devices. Each beam represents a single bit of
memory. The storage density is inversely proportional to the area occupied by each beam, so the ideal array would use the smallest beams possible. The data is then “written” by buckling the beams. A downward-buckled beam is a “1” and an upward-buckled beam is a “0”.

Beam (a) is in the initial, unbuckled state. Beam (b) is being heated, either through a thin-film resistor, or a heated tip designed as a writing device, at a constant rate.

![Figure 5.9 Nano-mechanical memory actuation in a memory array](image)

After a time $t_b$, the thermal stresses in the axial direction $x$, will cause the compression force in the beam to exceed the force required for buckling as shown in Eq. (5.10), causing the beam to buckle down as shown in (c). The temperature gradient in the beam at the moment of buckling is shown in Figure 5.10. The top layers are at higher temperature due to the heat addition to the top of the beam. This causes the top layers to expand more creating a downward bending moment in negative $z$ direction. If the heat is added to the bottom of the beam, the temperature gradient will be reverse and the beam will buckle up as (d) which corresponds to a “0”. According to the stability of the buckled structure, beams (c) and (d) stay buckled without the need of a sustaining heat (Arya et al., 2006). Hence, the device is a non-volatile memory.
Figure 5.10 Cross sectional temperature distribution ($T_w - T$) at the time of buckling

The data can be read and write and erased using a thermo-mechanical scanning-probe cantilever (Vettiger et al., 2002). The scanning probe cantilever was used to read and write the data in a thermomechanical memory with a totally different operation from the suggested memory in this study. Figure 5.11 shows the schematics corresponding to writing (see a) and reading (see b) process using scanning-probe cantilever. The writing process is a combination of applying a local force by the cantilever/tip to the polymer layer and softening it by local heating. Initially, the heat transfer from the tip to the polymer through the small contact area is very poor and improves as the contact area increases. This means the tip must be heated to a high temperature about 400 C to initiate the softening. Once softening has commenced, the tip is pressed into the polymer, which increases the heat transfer to the polymer, increases the volume of softened polymer, and hence increases the bit size. The exact writing process by Vettiger is not used in the writing procedure of the suggested memory, but the idea can be used to add the required heat to buckle the bit without pressing the tip to the memory bit.
The thermal conductance between the heater platform and the storage substrate changes according to the distance between them. This principle was used by Vettiger to read the data as shown in Figure 5.11 (see b). The medium between a cantilever and the storage substrate for example air, transports heat from one side to the other. When the distance between the heater and sample is increased as the tip moves into a bit indentation, the heat transport through air will be more efficient, leading to a decrease in the heater’s temperature and its resistance. Thus, changes in temperature of the continuously heated resistor are monitored while the cantilever is scanned over data bits, providing a means of detecting the bits. Vettiger increased the readback speed up to 1 Mb/sec by using an array of 32 by 32 scanning cantilever. In the suggested memory the scanning probe can move over the array of memory beams and report “0” and “1” based on the heaters’ resistance variations facing the buckled up to buckled down beams. While the Vitteger thermo-mechanical system is not erasable, the suggested buckling beam memory is erasable by re-positioning all the bits buckled up as shown in d. As previously explained, this position represents “0”.
The required buckling energy and buckling temperature can be estimated theoretically for a single bit of memory. The geometry and boundary conditions for complete and simplified geometries are illustrated in Figure 5.12. A single bit of memory is a doubly clamped bridge as shown in Figure 5.12 with fixed-fixed boundary conditions.

The critical buckling load can be rewritten as follows, using Eq. (5.10) (Timoshenko and Goodier, 1951):

$$ P_{cr} = EI \left( \frac{\pi}{\kappa L} \right)^2, $$

(5.11)

where $E$ is the modulus of elasticity, $I$ is the moment of inertia, $L$ is the length of the bridge and $k$ is the column effective length factor equivalent with $L_e/L$ as shown in Figure 5.4 which is equal to 0.5 for a bridge with fixed ends.

![Figure 5.12 Geometry (a) Complete model (b) Simplified model](image)

The thermal force due to thermal stress is calculated using the following formulation (Boley and Weiner, 1960):
\[ F_{th} = \iiint_{\text{Area}} \alpha E \cdot (T-T_w) \cdot dy \cdot dz \quad (5.12) \]

where \( \alpha \) is the thermal expansion coefficient, \( T \) is the temperature distribution, and \( T_w \) is the wall temperature.

In an ideal case, where there are no losses to the surrounding material or the gas, and the temperature inside the bridge is uniform, Eq. (5.12) simplifies to:

\[ F_{th} = A_c \alpha \cdot E \cdot (T_b - T_w) \quad (5.13) \]

where \( T_b \) is the total required buckling temperature, and \( A_c \) is the cross section of the beam. \( T_b \) can be found by equating the formulation for thermal stress inside the beam (Eq. (5.13)) with the critical buckling load (Eq. (5.11)):

\[ T_b = \left( \frac{\pi d}{L} \right)^2 \cdot \left( \frac{1}{3\alpha} \right) + T_w \quad (5.14) \]

Using Eq. (5.14) the required buckling energy with uniform volumetric heating with no conduction is obtained as:

\[ Q_v = \left( \frac{\pi^2}{3} \right) \cdot \left( \frac{\rho \cdot c_p}{\alpha} \right) \cdot \left( \frac{W \cdot d^3}{L} \right) \quad (5.15) \]

where \( \rho \) is the density, \( c_p \) is the specific heat, \( W \) is the width, \( d \) is the thickness, and \( L \) is the length of the bridge as shown in Figure. 5.12. In order to investigate the surface-heating case with conduction losses, there is a need to perform the simulations.

Unintentional heat addition to the beam structure in the device can cause accidental buckling or a bit flip, which either scrambles the data or erases it. In the highly radioactive environment of space, high energy protons and electrons may strike the structure. These particles can be a result of solar events or the planetary environment (Fortescue et al., 2003). High energy particle collision will add an instantaneous high energy to the beam structures. To avoid accidental resetting of the
spacecraft memory, the beam must be sized so that the energy of the particles does not cause buckling.

5.3 Simulation

The single material strategy is selected in the simulations. This means the buckling beam consists of a thin material instead of layers of various materials with different thermal expansion coefficients (sandwich structure) as described in section 5.2.2. Apparently, the layers with higher thermal expansion coefficient accelerate the buckling. This means single layer simulation overestimates the write time of the device. Since this study is limited to estimate the write time and the power consumption of the device, not the memory operation, single material simulation is acceptable as the worst scenario case.

Furthermore, the material properties are assumed constant at the wall temperature as shown later in Table 5.1. This assumption does not seem feasible at the first glance. For example, silicon conductivity drastically decreases by the temperature (Hull, 1999). But the structure reaches to the critical buckling force faster at a lower conductivity. As a result, these simulations overestimate the write time of the device which is acceptable as another worst selected scenario.

Figure 5.12 (see a) shows the complete geometry which must take into account the mountings. There are two mountings with the length l and the width w added to the beam. The mountings are fixed and have the constant temperature \( T_w \) at the bottom and two ends. However, simplified geometry does not simulate heat transfer in the mountings as shown in Figure 5.12 (see b). The beam is of length L, width W, and depth d, and is at an initial temperature \( T_w \). Depending on how the device is packaged, it may be surrounded by gas molecules at \( T_a \), and have a convective heat transfer coefficient \( h \). For thermal actuation in both models, the heat load is assumed to be applied on the top of the beam, at a rate of \( q'' \) (in Watts/m\(^2\)).
5.3.1 Buckling Simulation

As the temperature of the beam increases, the thermal stresses in the beam will increase until the axial force reaches the force required for buckling as explained in the previous section, and the beam will buckle. To capture this process, the transient heat conduction equation inside the beam must be solved which is given as Eq. (2.1):

\[
\frac{\partial T(x, y, z, t)}{\partial t} = \frac{k}{\rho c_p} \left( \frac{\partial^2 T(x, y, z, t)}{\partial x^2} + \frac{\partial^2 T(x, y, z, t)}{\partial y^2} + \frac{\partial^2 T(x, y, z, t)}{\partial z^2} \right)
\]

(2.1)

The boundary conditions are based on the thermal conditions at the surface and ends of the beam. There are three different types of boundary condition in this model (Figure. 5.12): One Dirichlet boundary condition and two types of Neumann boundary conditions. The Dirichlet boundary condition is defined as Eq. (2.12):

\[
T = T_w.
\]

(2.12)

The Neumann boundary condition applied to the heated surfaces is defined as Eq. (2.13) and the Neumann boundary condition applied to the unheated surfaces is defined as Eq. (2.14) as previously explained in section 2.3 of chapter 2:

\[
-k \frac{\partial T}{\partial n} = h(T - T_a) + q^\prime
\]

(2.13)

\[
-k \frac{\partial T}{\partial n} = h(T - T_a)
\]

(2.14)

The heat transfer coefficient, \( h \) is calculated based on the free molecular theory for an ideal gas. The formulation is given in Eq. (2.17) of section 2.4 in chapter 2:

\[
h = \sigma_T n_i \frac{\gamma + 1}{\gamma - 1} \sqrt{\frac{k_n T_a}{8\pi m}}.
\]

(2.17)
where $\sigma_T$ is the thermal accommodation coefficient, $\gamma$ is the specific heat ratio of the gas, $m$ is the molecular weight of the gas, and $n_i$ is the number density of the gas. For an ideal gas, $n_i$ can be calculated using

$$n_i = \frac{P_{\text{gas}}}{m \, RT_a},$$

where $R$ is the ideal gas constant.

The time-dependent temperature field will be used to find the thermal stresses in the beam. When the axial load due to the thermal stress is equal to the critical buckling load, the simulated beam is assumed to buckle (Chiao and Lin, 2000). The axial load is calculated using Eq. (5.12) where $T$ is the nodal temperature distribution. The formulation is applicable to the both models shown in Figure 5.12 because the mountings are fixed at the bottom.

A Finite Difference solver (Section 3.2.3, Chapter 3) that allows the temperature, materials, ambient conditions, heat load, and the geometry to be changed is used to solve these equations. Using these results, a buckling time, $t_b$ and a total energy for buckling $Q$ for any given geometry and ambient conditions are computed:

$$Q = t_b \cdot q^*,$$

where $q^*$ is the total heating rate added to the top:

$$q^* = W \cdot L \cdot q''.$$ 

### 5.3.2 High Energy Particle Collision

As previously explained in sections 5.1 and 5.2, high energy protons and electrons may strike the structure in the highly radioactive environment of space. The high energy particle bombardment is not continuous. For example, the integral flux is given as 100 particles per cm$^2$-s for electron bombardment and 10 particles per cm$^2$-s for proton bombardment in Europa orbit of
Jupiter (Jun and Garrett, 2005). This means the possibility of electron collision in this environment for a bit of 10 micron length and 1 micron width is 6 electrons per week. This value decreases to 2.4 proton per month for proton bombardment. Although the frequency of collisions is low, the spacecraft may have to store information, such as the operating system, for years. Therefore, the system must be designed not to buckle after high-energy collisions.

In order to simulate high energy particle collisions, it is assumed that only one particle hits the top surface in the center. The particle is small enough to add an instantaneous heat to the central node at the top surface. The amount of this heat depends on the energy the particle carries. The high temperature is calculated assuming the entire energy is transferred to a node:

\[ T_{hep} = \frac{E_{hep}}{\rho \cdot c_p \cdot \delta x \cdot \delta y \cdot \delta z} + T_w, \quad (5.18) \]

where \( E_{hep} \) is the energy of the corresponding high energy particle, \( \delta x, \delta y, \) and \( \delta z \) are the space discretizations in the x, y, and z directions respectively. The same Finite Difference solver is used to investigate the probability of the buckling at the time of collision. The rate of heat dissipation is also calculated using the same solver.

### 5.4 Results

Numerical simulations are performed to study the effects of various geometry dimensions, material properties and heating rate on the write time of the device which is called buckling time. Radiation resistance of memory bits in high radiation environment is studied for various materials.

The primarily simulations are performed with silicon because it is easy to micro-fabricate and has been integrated with IC circuits. The study continues with four more materials: silicon carbide, PMMA, parylene and kapton (Table 5.1).
5.4.1 Geometry Optimization

There are five input parameters and two output parameters determining the optimized geometry. The input parameters are the length, \( L \), the width, \( W \), and the thickness, \( d \), of the memory bit beam and the mountings length \( l \) and the width \( w \). The output parameters are the buckling time and required energy. The objective of the geometry optimization is to optimize input dimensions to minimize both output parameters: buckling time and required energy.

5.4.1.1. Beam Optimization. In order to investigate how the buckling time changes with the mounting length and width, the buckling time is obtained for the complete model with beam length of 20 \( \mu \text{m} \), width of 1 \( \mu \text{m} \) and the thickness of 300 nm and various mountings widths and lengths. The results are compared with those of simplified model. Figure 5.13 (see a) shows the buckling time for various mounting dimensions and the simplified model. The results are in agreement for the mountings dimensions up to 5 \( \mu \text{m} \). These results show the single bit study can be performed using the simplified model and also the mountings dimension has no effect on the write time of the device.

Figure 5.13 (see b) shows the buckling time variations versus total heating rate at the top of the bridge for silicon using the simplified model. As the length of the beam increases the buckling time decreases. This shows longer structures buckle faster and return a smaller writing time. The buckling time decreases as the total heat added to the top increases. This means the writing time become faster by increasing the heat addition to the top of the beam.

Figure 5.14 shows the required energy variation with the total heating rate at the top. Calculations show that for a bridge with the length of 20 microns, width of 1 micron and the thickness of 300 nm, the least total energy of 2.06 nJ is required to buckle the bridge. This value is smaller than the estimated value of 3.96 nJ calculated using Eq. (5.15). Longer structures will buckle at lower temperatures, and will require less energy to actuate. If a ratio of calculated
surface-heating energy divided by uniform volumetric heating energy is defined, this ratio remains constant around 51% for all the beam lengths with the same thickness and width.

Figure. 5.13 Buckling time variations by total heat added to the top (silicon) (a) Complete model for L=20 μm (b) Simplified model

Although the required energy to buckle for a beam with constant dimensions is expected to be constant, it slightly decreases as the total heating rate at the top increases. It shows it is more efficient to add more heat and make the buckling faster. The faster buckling does not increase the losses.
Figure 5.14 Required energy versus total heating rate (silicon)

Figure 5.15 shows the buckling time variations by thickness for silicon-bridge, with two different lengths of 20 and 40 microns. As the thickness of the bridge increases, the energy consumption increases due to an increase in the moment of inertia (Eq. (5.11)) leading to an increase in the buckling time. The graphs show that the buckling time for the same length decreases to the half as the total heating rate increases twice. The graph for the length of 20 microns and the total heating rate of 124 mW and the graph for the length of 40 microns and the total heating rate of 62 mW approximately collapse. These results show the buckling time changes inversely with the beam length and total heating rate.

Figure 5.15 Buckling time versus thickness for varying total heating rates (Silicon)
Figure 5.16 shows the buckling time variation by width for the silicon bridge. An increase in the width leads to an increase in the moment of inertia. As a result, the behavior of Figure 5.15 is expected. The buckling time increases as the width increases.

![Figure 5.16 Buckling time versus width (Silicon)](image)

5.4.1.2. Spacing Optimization. Writing at high data rates will require that there be no cross-talk between bits when they are written on in parallel. The most extreme case is writing on all of the bits bordering a bit that is not being used. Figure 5.17 shows an unheated bit surrounded by heated bits in an array of 3 in 3 bits. The unheated bit is at initial temperature $T_w$ and supposed to stay unbuckled. Buckling of the unheated bit due to heat conduction from the heated bits will compromise the data and must be avoided. To investigate if undesired buckling happens, the maximum possible heat flux is applied to the unheated beam’s mountings at the sides. The result shows that the unheated beam does not buckle and the centerline temperature is much smaller than the buckling temperature. In a silicon beam, the centerline temperature is 292.1 K while the buckling centerline temperature is 570 K. The study is performed for a range of spacing between 0.5 and 5 microns. The spacing of 0.5 microns is large enough for fabrication and avoiding undesired buckling.
5.4.2 Material

Table 5.1 shows the list of materials used for the study including thermal and mechanical properties at initial temperature 290 K. All of these materials are commonly used in microfabrication, making them suitable candidates for this device design. After obtaining the initial simulations for silicon, the study continues with silicon carbide. Silicon carbide has a higher melting point than silicon making it more appropriate for the harsh environments. Plastic materials are appropriate for mass fabrication. Two arbitrary plastic materials, PMMA and parylene, are selected for the preliminary plastic study. The material study terminated with kapton which has a low thermal conductivity and a high expansion coefficient, like other plastic materials, but will last for a longer time in high radiation environments.

<table>
<thead>
<tr>
<th></th>
<th>Kapton</th>
<th>Parylene</th>
<th>PMMA</th>
<th>Silicon</th>
<th>Silicon carbide</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ $(W/m\cdot K)$</td>
<td>0.12</td>
<td>0.02</td>
<td>0.25</td>
<td>130</td>
<td>120</td>
</tr>
<tr>
<td>$c_p$ $(J/Kg\cdot K)$</td>
<td>1090</td>
<td>711.75</td>
<td>1270</td>
<td>1000</td>
<td>750</td>
</tr>
<tr>
<td>$\rho$ $(Kg/m^3)$</td>
<td>1420</td>
<td>1289</td>
<td>1190</td>
<td>2330</td>
<td>3100</td>
</tr>
<tr>
<td>$\alpha$ $(1/K)$</td>
<td>$20\times10^{-6}$</td>
<td>$35\times10^{-6}$</td>
<td>$50\times10^{-6}$</td>
<td>$2.62\times10^{-6}$</td>
<td>$4\times10^{-6}$</td>
</tr>
<tr>
<td>$E$ $(Pa)$</td>
<td>$2.5\times10^{9}$</td>
<td>$400\times10^{3}$</td>
<td>$3\times10^{9}$</td>
<td>$130\times10^{9}$</td>
<td>$410\times10^{9}$</td>
</tr>
<tr>
<td>Melting point $(K)$</td>
<td>N/A</td>
<td>563</td>
<td>433</td>
<td>1683</td>
<td>3103</td>
</tr>
</tbody>
</table>
Figures 5.18 and 5.19 show the buckling time and required energy to buckle for five materials: silicon, silicon carbide, PMMA, parylene, and kapton. Silicon carbide buckles slightly faster than silicon because of its larger thermal expansion coefficient. PMMA, parylene, and kapton buckle much faster than silicon and silicon carbide because their expansion coefficients are an order of magnitude larger than silicon and silicon carbide’s ones. These three materials also require the least energy to buckle.

Figure 5.18 Buckling time for various materials

Figure 5.19 Required energy for various materials
5.4.3 High Radiation Collision

The trapped electron and proton energy spectra were previously obtained using the radiation belt models for the Europa orbit of Jupiter. It shows the highest energy and the most probable trapped electrons and trapped protons carry 1000 Mev and 100 Mev, respectively (Jun et al., 2005).

Figure 5.20 shows the heat dissipation of a bit with the length of 20 microns, width of 1 micron, and the thickness of 300 nm which is hit by the highest energy electron and proton at the top face. If buckling occurs it must be at the very beginning of the collision. The silicon simulation results show that the buckling does not occur. In addition, the heat due to the collision dissipates in less than 10 nsec which is much less than the quickest silicon bit buckling time for the same dimensions, 17 nsec.

![Graph showing heat dissipation over time for high energy electron and proton](image)

Figure. 5.20 Heat dissipation in a bit of memory after high energy particle collision (silicon)

Figure 5.21 shows the heat dissipation of silicon, silicon carbide, PMMA, parylene and kapton beams which are hit by the highest energy proton (see a) and electron (see b) at the center of the top surface respectively. Because of the relative infrequency of these collisions, the collision is modeled as a discrete heat addition at the most vulnerable point of the system, instead of a continuous heating. The heat dissipation in silicon carbide is slightly different from silicon while it is much slower in PMMA, parylene, and kapton because of the small thermal conductivity. In
electron collision, the force due to thermal stresses pass the required buckling force leading to undesired buckling in PMMA, parylene, and kapton beams. However, in the proton collision case, the thermal force does not exceed the required buckling force to buckle the PMMA, parylene, and kapton beam.

Table 5.2 shows the critical buckling force required to buckle a beam with a length of 20 microns for silicon, silicon carbide and kapton. The critical buckling force is calculated using Eq. (5.11). The critical buckling force required to buckle a kapton beam is two order of magnitude
smaller than silicon and silicon carbide due to the smaller modulus of elasticity as shown in Table 5.2.

Figure 5.22 shows the thermal force decay in the beams due to high energy proton collision (see a) and high energy electron collision (see b). The results show that silicon and silicon carbide beams are radiation resistant in both high energy electron and proton collisions. In electron collision, the force due to thermal stresses pass the required buckling force leading to an undesired buckling in kapton beam. However, in the proton collision case, the thermal force does not exceed the required buckling force to buckle the kapton beam.

![Figure 5.22 Force decay in a bit of memory after (a) proton collision (100 Mev) (b) electron collision (1000 Mev)](image)
Table 5.2 Critical buckling force

<table>
<thead>
<tr>
<th></th>
<th>Kapton</th>
<th>Silicon</th>
<th>Silicon carbide</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_c$ (nN)</td>
<td>444</td>
<td>23,095</td>
<td>72,838</td>
</tr>
</tbody>
</table>

5.4.4 Pressure Effects and Packaging

Previous studies showed the pressure and dimension variations in packaging will change the heat transfer coefficient $h$ (Masters et al., 2005; Lee et al., 2007). This has the potential to change the write time of the device. Previous researchers have studied the heat transfer in vacuum packaged systems. This work has included modeling of gas phase conduction heat transfer between a substrate and a cantilever leg at constant temperature in the free molecular flow regime (Masters et al., 2005). A related work shows air pressure increase will raise the dissipated power in a heated microcantilever (Lee et al., 2007). In both cases, the low pressure and small length scales showed that free-molecular models for heat transfer are appropriate.

Pressure variations appear in heat transfer coefficient variations as given in Eq. (2.17) and Eq. (2.18). Increasing the pressure leads to an increase in heat transfer coefficient and dimensionless Biot number, $hl/k$. In this study, all the results shown in Figures 5.13 to 5.22 are obtained at constant pressure 5 kPa which yields Biot numbers of 35.25, 205.53, 16.44, 0.0316, and 0.034 for kapton, parylene, PMMA, silicon, and silicon carbide, respectively. Plastic materials show larger Biot numbers in comparison with silicon and silicon carbide.

Figure 5.23 shows the buckling time variations by the pressure increase for a bit of kapton and silicon carbide. Kapton shows larger buckling time as the pressure passes 100 Pa. However, the buckling time remains constant for silicon carbide. This behavior can be explained using Biot numbers. Kapton has a large Biot number while silicon carbide has a Biot number 1000 times
smaller than Kapton. Previous studies show that the center displacement variation for a heated bridge is significant at high Biot numbers (Maghsoudi and Martin, 2012a).

![Graph showing writing time variations with pressure](image)

Figure. 5.23 Air pressure effects on writing time variations (logarithmic scale)

### 5.5 Conclusion

The energy required for writing data per bit is in the order of 1 nJ which shows low power consumption of the device. The data storage density is a trade-off. In order to balance these constraints, the length of 20 microns and the smallest possible thickness to fabricate, is suggested. This design suggests a memory density in the order of $10^6$ bits/cm$^2$ and $10^{11}$ bits/cm$^3$ which are acceptable in comparison with the current memory devices and can be improved by decreasing the width and the thickness of the beam.

Decreasing the thickness and the width is desired for both energy consumption and buckling time. However, decreasing the length has inverse effects. The buckling time changes inversely with the total heating rate and the length of the beam. The simulation results show that the write time of less than 10 nsec/bit is achievable (100 MB/sec). Because this technology allows reading and writing in parallel, the writing process can be accelerated using multiple reading/writing heads.
The results obtained of simulation a bit of memory including mountings are in agreement with the results of simplified model. The simplified model is a good approximation of the complete geometry.

PMMA, parylene, and kapton bits consume the least power and buckle faster than silicon and silicon carbide bits. However, electron collision causes undesired buckling in PMMA, parylene, and kapton bits. High energy particle collision will not lead to undesired buckling in the silicon and silicon carbide memory bits. The heat due to the collision dissipates in less than 10 nsec. As a result, either silicon or silicon carbide is the most appropriate material to fabricate the device for Jovian moon or other extreme environments. However, PMMA, parylene, and kapton are more appropriate alternatives for other missions where radiation environment is not extreme. The pressure variation and packaging affect the write time of plastic materials while do not change the write time in silicon and silicon carbide bits significantly.

Although the simulations reported acceptable writing time and power consumption for the suggested buckling memory, and confirmed a radiation protected design for harsh environments there are a few weaknesses associated with the simulations:

1. The thermal properties are assumed constant as the worst scenario case. Increasing the temperature will drastically decrease the thermal conductivity and increase the thermal expansion which accelerate the buckling resulting in smaller buckling time.

2. The single material strategy is selected while it has the tendency to become mono-stable eventually. Sandwich materials reported as bistable membranes are more appropriate approach for the simulations.

3. The writing time was not taken the probe speed into account. This becomes very important especially because two arrays of writing probes are required: one at the top and another at the bottom of the array of buckling memory.
The simulations can be significantly improved by using the temperature dependent thermal properties solver for heat conduction equation. However, this will show a smaller writing time while the current writing time falls within a reasonable range. Fabrication and preliminary tests on a single bit of buckling memory can provide necessary information for the continuation of the simulations and determine the necessity of using a sophisticated structural formulation.
CHAPTER 6: TRANSIENT RESPONSE IN NANO-BRIDGES

As previously discussed in section 1.3 of the introduction, applying sinusoidal heating leads to vibration in the bridge called “thermal actuation”. This chapter simulates a three-dimensional doubly clamped bridge with the step function and harmonic heat addition. The simulation is only performed in nano-scale. Silicon is the selected material for the study. Only the free molecular approach is used to define the heat transfer and damping coefficients.

This chapter contains analysis of the step function response which determines the direction of deflection, the dominant frequencies in the system and settling time. The harmonic excitation study includes computing the phase delay between the excitation and the response, the steady state amplitude, and the vibration amplitude for a range of frequencies. It also discusses the changes of the vibration amplitude and the steady state amplitude for a range of pressures below the atmospheric pressure.

The transient heat transfer and structural equations are solved using a Finite Difference method implemented in C++. The implicit approach is used for constant thermal properties while the explicit approach is used for temperature dependent thermal properties.

6.1 Geometry and Boundary Conditions

The geometry is a nano-scale bridge as introduced in Chapter 2. Figure 2.1 shows the geometry which is a beam with a length of 10 microns, a width of 1 micron, and a thickness of 300 nanometers. Conduction within the beam and convection between the beam and the quiescent gas are considered. In contrary with chapter 2, the is doubly clamped.

For step function excitation, a constant heat flux $q^t$ is added to the top of the bridge uniformly. However, for harmonic excitation a time-dependent heat load is added to the system. If the system consists of a resistor, $R$, with current $I(t) = I_0 \times \sin(\omega t)$ passing through it, then the power can be
defined as $q = R[I_0 \times \sin(\omega_a t)]^2$. This means that the time-dependent harmonic heat load, $q''$, applied to the top surface of the beam can be expressed as follows:

$$q'' = A_h (\sin(\omega_a t))^2 = A_h [1 - \cos(\omega t)]$$

where $A_h$ is the heat load amplitude, $t$ is the time, and $\omega_a$ is the actuation frequency, and $\omega$ is the frequency of the system:

$$\omega = 2\omega_a$$  \hspace{1cm} (6.2)

The excitation frequency and the response frequency will be equal to $\omega$ because the “$\sin$” term raised to power 2 is equivalent with $(1-\cos(\omega t))$ as shown in Eq. (6.1). This is equivalent with an unbalanced harmonic excitation.

All other thermal boundary conditions except the heat load are preserved as thermal boundary conditions explained in chapter 2 (Figure. 2.1).

Figure. 2.1 The geometry and boundary conditions in the model

The cooling gas is air with constant properties at ambient temperature. Simulations are performed for crystalline silicon. The thermal properties of crystalline silicon are assumed to be constant and defined at the wall temperature in the implicit approach. Another approach updates the silicon thermal properties by temperature at each time step. The wall temperature, $T_w$, is fixed at both ends of the beam.
6.2 Transient Thermo-structural Formulation

6.2.1 Transient Heat Transfer Equation

For the constant thermal properties approach Eq. (2.1) is used:

\[
\frac{\partial T(x, y, z, t)}{\partial t} = \frac{k}{\rho c_p} \left( \frac{\partial^2 T(x, y, z, t)}{\partial x^2} + \frac{\partial^2 T(x, y, z, t)}{\partial y^2} + \frac{\partial^2 T(x, y, z, t)}{\partial z^2} \right),
\]

(2.1)

where \( k \) is the thermal conductivity of the solid. This equation is solved using an implicit Finite Difference approach at each time step to obtain the nodal temperature distribution when the thermal properties are assumed constant at the wall temperature.

However, for the temperature dependent thermal properties approach, Eq. (2.11) is used which takes into account the thermo-elastic terms and also temperature dependency of the thermal properties (Landau and Lifshitz, 1959; Lifshitz and Roukes, 1999; Serra and Bonaldi, 2008):

\[
\left( 1 + \frac{2E\alpha^2 T(x, y, z, t)}{\rho c_p} \right) \left( 1+\nu_p \right) \frac{\partial T(x, y, z, t)}{\partial t} = \frac{1}{\rho c_p} \left( \frac{\partial}{\partial x} \left( k \frac{\partial T(x, y, z, t)}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T(x, y, z, t)}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T(x, y, z, t)}{\partial z} \right) \right) \]

\[
+ \frac{E\alpha T(x, y, z)}{\rho c_p} \frac{\partial}{\partial t} \left( \frac{\partial^2 v(x, t)}{\partial x^2} \right),
\]

(2.11)

where \( \nu_p \) is the Poisson ratio and \( c_p \) is the specific heat.

The thermal boundary conditions are the same as chapter 2 from Eq. (2.12) to Eq. (2.14). There are three different types of boundary condition in this model (Figure 2.1). The Dirichlet boundary condition at both ends is expressed as:

\[ T = T_w. \]

(2.12)

There are two different types of Neumann boundary conditions which are applied to the heated and unheated surfaces. Equation (2.13) shows the boundary condition for the heated surface, and Eq. (2.14) shows the boundary condition for the unheated surfaces:

\[ n \cdot \left( k \frac{\partial T}{\partial n} \right) = 0 \]
The heat conduction equation is solved numerically using a Finite Difference method (Incropera et al., 2007). As a result, the temperature is obtained at each node. These results are used to calculate the thermal stress due to temperature differences in the beam and the thermal moment and force.

Only the free molecular approach is selected to compute the heat transfer coefficient, \( h \). The formulation is presented in section 2.4:

\[
h = \sigma_T n_i \frac{\gamma + 1}{\gamma - 1} \frac{k_b T_a}{8\pi m},
\]

where \( \sigma_T \) is the thermal accommodation coefficient, \( \gamma \) is the specific heat ratio of the gas, \( m \) is the molecular weight of the gas, and \( n_i \) is the number density of the gas. For an ideal gas, \( n_i \) can be calculated using

\[
n_i = \frac{P_{\text{gas}}}{m R T_a},
\]

where \( R \) is the ideal gas constant.

### 6.2.2 Transient Structural Equation

In this chapter, the transient structural equation, which takes into account the unsteadiness is used. The derivation of the equation is explained in chapter 2. The primary form of the equation is given as follows:

\[
\rho A \frac{\partial^2 \nu(x,t)}{\partial t^2} + \left( EA \left[ \frac{\partial u}{\partial x} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right] - N_{th} \right) \frac{\partial^2 \nu(x,t)}{\partial x^2} + \frac{\partial}{\partial x} \left( EI \frac{\partial^2 \nu(x,t)}{\partial x^2} + M_{th} \right) + F_D(x,t) = 0,
\]
where the damping term, $F_D$ is the net flow drag (Martin and Houston, 2008) in the free molecular regime. It is equivalent with the constant damping term, $C_f$ multiplied by vibration velocity. $F_D$ is given by:

$$F_D = \frac{W_P}{c} U(x,t) \left[ (2 - \sigma_n) \left( \frac{2}{\sqrt{\pi}} + 1 \right) + \sigma_n \sqrt{\pi} \left( \frac{T_w}{T_a} + 2 \frac{d}{W} \frac{\sigma_t}{\sqrt{\pi}} \right) \right] = C_f U(x,t),$$

(2.30)

where $\sigma_n$, the normal accommodation coefficient and $\sigma_t$, the tangential accommodation coefficient are assumed to be equal to 1. The thermal velocity, $c$, is defined in Eq. (2.31), and $U(x,t)$ is the velocity in the vibration direction, $z$ which is defined as Eq. (2.32):

$$c = \sqrt{\frac{2k_bT_a}{m}},$$

(2.31)

$$U(x,t) = \frac{\partial v(x,t)}{\partial t},$$

(2.32)

where $m$ is the mass of the gas molecules, in this case air with $m=481.1 \times 10^{-27}$ kg. Other terms, $k_b$ and $T_a$ are previously defined in chapter 2 as Boltzmann constant and ambient temperature.

Substituting Eqs. (2.30) in Eq. (2.29), the finalized dynamic structural equation is obtained:

$$\rho A \frac{\partial^2 v(x,t)}{\partial t^2} + \left( EA \left[ \frac{\partial^2 u}{\partial x^2} + \frac{1}{2} \left( \frac{\partial v}{\partial x} \right)^2 \right] - E \int \alpha(T - T_w)dydz \right) \frac{\partial^2 v(x,t)}{\partial x^2}$$

$$+ \frac{\partial}{\partial x} \left( EI \frac{\partial^2 v(x,t)}{\partial x^2} + E \int \alpha(T - T_w)zdydz \right) + C_f \frac{\partial v(x,t)}{\partial t} = 0.$$  

(2.33)

Equation (2.33) is solved numerically using a Finite Difference method to obtain the displacement along the bridge. The presence of the fourth-order derivative of the displacement with respect to $x$ in Eq. (2.33) requires two additional points other than both ends at the boundaries. To fulfill this requirement, two ghost points are created at both ends. The fixed-fixed boundary condition requires zero displacement and slope zero at both ends. Beginning the first time step, the following boundary condition is applied to both ends at all the time steps:
\[
\begin{align*}
\nu(x = 0, L, t) &= 0, \\
\frac{\partial \nu}{\partial x}(x = 0, L, t) &= 0.
\end{align*}
\tag{2.36}
\]

The discretization algorithm and solution method will be as discussed in section 3.2.3 of chapter 3. In this case, the slope zero boundary condition is applied using the ghost point. Figure 6.1 shows the computational points at the left end. The ghost point is labeled as “g” and the end point is numbered 1, the nodes numbers increase towards the other end point in the right.

![Figure 6.1 Computational nodes at the boundary](image)

Equation (6.3) shows the discretized form of Eq. (2.36) at each time step.

\[
\begin{align*}
\nu_1 &= 0, \\
\frac{\nu_g - \nu_2}{\Delta x} &= 0,
\end{align*}
\tag{6.3}
\]

where \(\nu_g\) is the displacement at the ghost point \(\nu_1\) is the displacement at the end point and \(\nu_2\) is the displacement at the first node next to the end point. This simply means that at each time step the governing transient structural equation Eq. (2.33) is solved at all the nodes except the two ends and the ghost points. At the end of each time step the slope zero boundary condition is satisfied by equating \(\nu_g\) with \(\nu_2\).

### 6.3 Validation of Unsteady Thermo-structural Equations

Although there is no set of analytical results to validate the coupled thermo-structural solver, the unsteady thermal solver and unsteady transient structural solver are validated independently to ensure the agreement with analytical solution. The unsteady thermal solver is validated for constant thermal properties. Later in this chapter, the constant properties thermal solver shows the same results as temperature dependent thermal properties solver at low temperatures.
In dynamic structural equation, the heat added to the system is set to zero which means no thermal bending moment or external force acts on the structure. Then, the beam is given the initial displacement corresponding to the first mode shape for fixed-fixed boundary condition. The results are validated using free vibration analytical solution.

### 6.3.1 Unsteady Thermal Equation Validation

In Chapter 3, the steady thermal equation was validated with analytical solution of uniform cross sectional rectangular fins. The results showed good agreement. In order to validate the unsteady conduction equation the analytical result of a long rectangular bar was used. Figure 6.2 shows a long rectangular bar with heat convection at the top, bottom, front and back sides.

![Figure 6.2 Long rectangular bar with convection at four sides (Yener et. al., 2008)](image)

The analytical solution for the temperature distribution by time in the cross section of the bar is given as (Yener et. al., 2008):

\[
\left[ \frac{T(y,z,t) - T_a}{T_w - T_a} \right]_{w} = \left[ \frac{T(y,t) - T_a}{T_w - T_a} \right]_{w} \times \left[ \frac{T(z,t) - T_a}{T_w - T_a} \right]_{d}, \tag{6.4}
\]

where \( T_w \) is the initial temperature since the bar is at wall temperature at time \( t=0 \), and \( T_a \) is the ambient temperature. The first and second term in the right hand side can be obtained using the following formulation:

\[
\left[ \frac{T(y,t) - T_a}{T_w - T_a} \right]_{w} = \sum_{n=1}^{\infty} C_n e^{-\xi_n^2 Fo} \cos \left( \xi_n \frac{y}{0.5W} \right), \tag{6.5}
\]

where \( Fo \) is the Fourier coefficient:
The coefficient $C_n$ is:

$$C_n = \frac{4\sin(\zeta_n)}{2\zeta_n + \sin(2\zeta_n)},$$

and the discrete values of $\zeta_n$ (eigenvalues) are positive roots of the transcendental equation:

$$\zeta_n \sin(\zeta_n) = Bi_w$$

$$= \frac{h(0.5W)}{k}.$$  \hspace{1cm} (6.8)

The first four roots of this equation are tabulated (Incropera et al., 2007). The second term in the right hand side of Eq. (6.4) can be calculated by substituting $W$ by $d$ in Eqs. (6.5) to (6.8).

In order to validate the numerical solution of constant thermal properties conduction equation Eq. (2.1) with analytical solution Eq. (6.4), a larger length of 25 micron was used which is 25 times larger than the width of 1 micron and 83 times larger than the thickness. Ambient temperature $T_a$ of 320 K was selected. Center temperature was tracked by time and plotted versus the analytical solution for various number of divisions along the x axis. The results are in agreement for 89 divisions along x axis as shown in Figure 6.3.

**Figure. 6.3 Center temperature (analytical versus numerical solution)**
6.3.2 Unsteady Structural Equation Validation

In the dynamic structural equation as shown in Eq (29), if the heat is set to zero, the dynamic structural equation for no external force will be as follows:

$$\rho A \frac{\partial^2 \nu(x,t)}{\partial t^2} + EI \frac{\partial^4 \nu(x,t)}{\partial x^4} = -C_f \frac{\partial \nu(x,t)}{\partial t}.$$  \hspace{1cm} (6.9)

The beam with no external force acting on it is given an initial displacement corresponding to the first mode shape for fixed-fixed boundary condition with $A_0$ of 1 nanometer as shown in Figure 6.4. The initial displacement is calculated using the following formulation over half of the beam (Martin and Houston, 2009):

$$\nu(x,0) = 0.630A_0 \left\{ -1.00 \left[ \cos \left( \frac{4.73}{L} x \right) - \cosh \left( \frac{4.73}{L} x \right) \right] ight. $$

$$\left. + 0.9852 \left[ \sin \left( \frac{4.73}{L} x \right) - \sinh \left( \frac{4.73}{L} x \right) \right] \right\}.$$ \hspace{1cm} (6.10)

![Figure. 6.4 Initial displacement](image)

The beam vibrates with air damping coefficient. If the damping coefficient was zero, the beam would vibrate with the natural frequency of the bridge $\omega_n$ which is given by (Timoshenko et al., 1974):
where $k_n$ is the mode constant which is equal to 4.694 for the bridge and $m$ is the mass per unit length ($\rho W d$).

Including damping coefficient, the system vibrates with damping frequency $\omega_d$ which is given as follows for $\xi<1$:

$$\omega_d = \omega_n \sqrt{1 - \xi^2},$$

where $\xi$ is the corresponding non-dimensional damping coefficient which is a function of the air pressure and ambient temperature. The quality factor, $Q$ is the ratio of the stored energy of the system to the dissipation energy:

$$Q = \frac{2\pi U_i}{U_d},$$

where $U_i$ is the stored vibrational energy in the system and $U_d$ is the energy dissipation per period (Blom et al., 1992).

For this model, the quality factor, $Q$ is equal to fluidic quality factor, $Q_F$ because the losses are dominated by gas losses. If the flow is free-molecular the following equation holds (Martin and Houston, 2008):

$$Q_F = \frac{k_m^2}{k_m \rho E} \left( \frac{d}{L} \right)^2 \left( \frac{\rho E}{12} \right),$$

where $k_m$ is given by:

$$k_m = \sqrt{\frac{m}{2k_n T_a}} \left[ 2 - \sigma_n \left( \frac{2}{\sqrt{\pi}} + 1 \right) + \sigma_n \sqrt{\pi} \left( \frac{T_m}{T_a} + 2 \frac{d}{W \sqrt{\pi}} \right) \right].$$

The damping coefficient, $\xi$ is defined using the following formulation:
\[ \xi = \frac{1}{2Q_f} \]  
\hspace{1cm} (6.16)

At 500 kPa the corresponding damping coefficient is \( \xi = 0.026 \).

The analytical solution for the system of equation is given as follows (Timoshenko et al., 1974):

\[ v(t) = e^{-\xi \omega_d t}\left( b_0 \cos(\omega_d t) + \frac{b_0 \xi \omega_d + v_0}{\omega_d} \sin(\omega_d t) \right), \]  
\hspace{1cm} (6.17)

where \( b_0 \) is the initial center displacement and \( v_0 \) is the initial displacement derivative with respect to time.

The analytical decay by time is given as follows (Timoshenko et al., 1974):

\[ v(t) = A_0 e^{-c_{t/2} \rho A}. \]  
\hspace{1cm} (6.18)

The numerical results were plotted versus analytical solution and the analytical decay as shown in Figures 6.5 to 6.7. The dotted plot refers to Eq. (6.18) and the dashed plot refers to Eq. (6.17). As the discretization along the beam becomes finer, agreement between the numerical and analytical solution is achieved.

![Figure 6.5 Numerical versus analytical solution for 7 computation nodes along the beam (NnodX=7)](image-url)
Figure 6.6 Numerical versus analytical solution for 15 computation nodes along the beam (NnodX=15)

Figure 6.7 Numerical versus analytical solution for 21 computation nodes along the beam (NnodX=21)

The accuracy is defined as the difference between the analytical and numerical solution at the last time step. Figure 6.8 shows the accuracy variations by the number of divisions along the beam. Since the displacement is in the order of nano in the validation study, for 7 divisions along the beam the accuracy is within the first significant digit. As the number of divisions increases the accuracy of up to fourth significant digit is achieved. This shows that the analytical and numerical solution are in agreement for 17 and 21 nodes along the beam.
6.4 Temperature Dependent Thermal Properties

The studies in chapters 3, 4, and 5 were performed assuming constant thermal properties at the wall temperature. However, as the structure is heated the temperature raise makes significant changes in the thermal properties such as thermal conductivity $k$, specific heat $c_p$ and thermal expansion coefficient $\alpha$. Figures 6.9 to 6.11 show crystalline silicon thermal properties by temperature variations (Hull, 1999).
Using the tabulated thermal properties versus temperature (Hull, 1999), thermal properties deviation by temperature is calculated as shown in Table 6.1.

<table>
<thead>
<tr>
<th>Temperature raise</th>
<th>40 K (from 290 K to 330 K)</th>
<th>100 K (from 300 K to 400 K)</th>
<th>300 K (from 300 K to 600 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deviation in thermal conductivity</td>
<td>15%</td>
<td>32%</td>
<td>59%</td>
</tr>
<tr>
<td>Deviation in thermal expansion coefficient</td>
<td>11%</td>
<td>24%</td>
<td>47%</td>
</tr>
<tr>
<td>Deviation in specific heat</td>
<td>4%</td>
<td>10%</td>
<td>19%</td>
</tr>
</tbody>
</table>
The thermal conductivity variations due to the temperature raise is significant. The temperature raise of 100 K decreases the thermal conductivity over 32%. The thermal expansion coefficient variations due to the temperature increase is less significant than thermal conductivity but is not negligible for higher temperature raise. The specific heat shows the least variations due to the temperature increase.

Table 6.1 shows the crystalline silicon thermal properties are highly temperature dependent. As the temperature increases beyond 100 K, the constant thermal properties assumption will be limited in predicting the thermo-structural behavior of the system. In order to take into account the temperature dependency of thermal properties, three subroutines are added to the explicit computational code which update the thermal properties at each time step using the provided tabulated data for crystalline silicon thermal properties versus temperature (Hull, 1999). As a result, the thermal conductivity, thermal expansion coefficient and specific heat are updated at each time step based on the corresponding discretized temperature domain at that time step.

6.5 Sensitivity Study

Term sensitivity study over unsteady conduction equation for variable thermal properties Eq. (2.11) is performed. The explicit temperature dependent thermal properties solver is run with and without thermo-elastic terms. The results show that the thermo-elastic terms create a difference up to the third significant digit in the temperature distribution. This is obtained for the total temperature raise of 100 K. However, Eq. (2.11) is solved as full in the rest of the study.

Term sensitivity study is also performed over the transient dynamic structural equation as shown in Eqs (2.29) and (2.33). The equation is solved once with the axial force term and another time without the axial force term for a constant distributed heat load of 50 mW added to the top of the beam. Figure 6.12 shows the center displacement versus time in both models. The small difference shows the axial force term does not have significant impact on the overall results.
In order to check the order of magnitude of the force and moment terms is Eq. (2.29) or (2.33), these terms are calculated using the thermo-structural solver for the full equation. The thermo-structural equation is solved including all terms presented in Eq. (2.29) or (2.33). A constant distributed heat load of 50 mW is added to the top of the beam. Figure 6.13 shows the logarithmic scale of absolute values of the total axial load and the thermal moment term. We used the absolute values so we can apply the log function. Because the values are very small, they were multiplied to $10^{20}$ while saving. The results show that the smallest values of the thermal moment term, are 2 order of magnitudes larger than the largest values of the axial load term, and the largest values of the thermal moment term, are 4 to 5 order of magnitudes larger than the largest values of the axial load term.
Figure 6.13 Logarithmic scale of absolute values of axial and thermal moment terms

Figure 6.14 plots the thermal moment term \( B \) divided by the axial load term \( A \) in logarithmic scale. Note that terms \( B \) and \( A \) are shown in Figure 6.13. This figure shows clearly that the thermal moment term is 2 to 5 order of magnitudes larger than the axial load. As a result, the axial load term can be ignored in comparison with the thermal moment term as previously done by other researchers (Lifshitz and Roukes, 1999).

![Graph showing logarithmic scale of absolute values of axial and thermal moment terms.](image)

Figure 6.14 Logarithmic scale of relative order of the thermal moment to the axial load term

scaling analysis was used as a mathematical tool to estimate the order of magnitude of term \( A \), the axial load term in comparison with term \( B \), the thermal moment term. Using Eqs (2.28) and (2.29) term \( A \) can be scaled as follows:

![Graph showing logarithmic scale of relative order of the thermal moment to the axial load term.](image)
\[
N \frac{\partial^2 \nu(x,t)}{\partial x^2} \propto \left[ EdW \left( \frac{u_0}{L} + \frac{1}{2} \left( \frac{u_0}{L} \right)^2 \right) - E \alpha \Delta T \, dW \right] \frac{u_0}{L^2},
\]

Using Eqs. (2.25) and (2.29), term B can be scaled as follows:

\[
\frac{\partial^2 M_{bb}(x,t)}{\partial x^2} \propto \left[ E \alpha \Delta T \frac{d^2}{2} \right] \frac{1}{L^2},
\]

where in Eqs (6.19) and (6.20), E is the modulus of elasticity, d is the thickness, W is the width and L is the length of the beam. \( u_0 \) is the maximum deflection which is in the order of nanometer, \( \Delta T \) is the maximum temperature difference, and \( \alpha \) is the thermal expansion coefficient. In order to compare the order of magnitudes of terms A and B, Eq. (6.19) is divided by Eq. (6.20). After canceling the same terms, \( A/B \) becomes:

\[
\frac{A}{B} \propto \frac{\left[ \frac{u_0}{L} + \frac{1}{2} \left( \frac{u_0}{L} \right)^2 \right] \frac{u_0}{L^2}}{\left[ \alpha \Delta T \frac{d}{2} \right] \frac{1}{L^2}} = \frac{\alpha \Delta T u_0}{\alpha \Delta T \frac{d}{2}}.
\]

Since \( u_0 \) is in the order of nanometer and L is 10 micrometer, \( l \gg u_0 \). As a result, \( u_0/L \gg (u_0/L)^2 \). Eq (6.21) can be rewritten as follows:

\[
\frac{A}{B} \propto \frac{\left[ \frac{u_0}{L} \right] \frac{u_0}{L}}{\left[ \alpha \Delta T \frac{d}{2} \right] \frac{d}{2}}.
\]

If the values of each scaled term is substituted in Eq. (6.22):

\[
\frac{A}{B} \propto \frac{\left[ \frac{10^{-9}}{10 \times 10^{-6}} \right] 10^{-9}}{\left[ 2 \times 10^{-6} (200) \right] \frac{300 \times 10^{-9}}{2}} - \frac{\left[ \frac{10^{-9}}{300 \times 10^{-9}} \right]}{\frac{10^{-9}}{2}} \propto 2 \times 10^{-3} - 6 \times 10^{-3}.
\]
Equation (6.23) shows for the current dimensions, term A can be ignored in comparison with term B. Using the results presented in Figures 6.12 to 6.14 and scaling analysis, the simulations used in this study do not take into account the axial load term in Eq. (6.33).

6.6 Results and Discussion

6.6.1 Step Function Excitation

In this section, step function excitation is applied to the transient thermo-structural equation for both the constant thermal properties solver and the variable thermal properties solver. A range of air pressures leading to a range of damping coefficients are used. Applying a constant heat flux to the system leads to vibration in the system but the system eventually converges to a constant center displacement. The study begins with higher pressure indicating a higher damping coefficients and continues with lower pressures.

6.6.1.1 Variable Properties Solver at 5 MPa Air Pressure. A constant distributed heat load of 50 mW is added at time \( t=0 \) to the top of the beam with the length of 10 micron, width of 1 micron and the thickness of 300 nm. The beam starts vibrating in the air with the pressure of 5 MPa corresponding to the dimensionless damping constant of \( \xi=0.26 \). Figure 6.15 shows the response, the negative center displacement by time. The response is plotted for three time durations as shown in green, red and blue. As shown in the blue plot the vibration is eventually damped to a constant center displacement value. The response plot shows the beam deflects downwards by adding the heat to the top of the structure. Adding the heat to the top of the structure creates a temperature gradient along the thickness of the beam. The larger expansion of the top layers due to the higher temperature increase will create a downward bending moment.
In order to track the temperature variations by time, the temperature at the top center of the beam was monitored by time. Figure 6.16 shows the top center temperature variations by time corresponding to green, red and blue response plots shown in Figure 6.15. The results show that the response is thermally steady state at the end of each set of simulations. This means the temperature distribution becomes identical at the last time step of the first run.

In order to study the relation between the temperature distributions along the beam with the corresponding deflected shape, temperature distribution and displacement along the beam are
plotted at the last time step of each response plot shown in Figures 6.17 and 6.18. Figure 6.17 shows the top center-line temperature distribution along the x axis. Figure 6.18 shows the corresponding deflected shape of the beam where point “1” represents the results at the last time step of the green plot, point “2” represents the results at the last time step of the red plot and point “3” represents the results at the last time step of the blue plot shown in Figures 6.15 and 6.16. An identical temperature distribution along the beam is obtained because as shown in Figure 6.16, the thermal equation becomes steady state at the corresponding 3 points. However, due to the dynamic effects, the displacement along the x axis is not identical in the last time step of each response simulation.

![Figure 6.17 Top center temperature distribution along the beam for a constant heat load of 50 mW at 5 MPa (Variable thermal properties)](image)

Figure 6.17 shows a sudden change in temperature at the edges. However, there is not a significant temperature gradient along the beam other than the edges. This creates a large bending moment close to the edges. As a result, as shown in Figure 6.18 a sudden change appears in the deflected shape close to the edges.
A Fast Fourier Transformation (FFT) code written in MATLAB is applied to the converged solution shown in Figure 6.15 in blue. This gives the dominant frequencies in the system. Figure 6.19 shows the dominant frequencies for the system. This shows that the system responds with all the modes for the step function excitation.

6.6.1.2. **Variable Properties Solver at 2 MPa Air Pressure.** This section presents the thermal and structural response of the beam with the same dimensions and heat load as section 6.6.1.1. The air pressure is decreased to 2 MPa corresponding to the dimensionless damping
constant of 0.104. Figure 6.20 shows the response by time for three time durations. In comparison with 5 MPa response, the settling time is longer for 2 MPa due to a smaller damping coefficient.

![Figure 6.20](image)

**Figure. 6.20 Response to constant heat load of 50 mW at 2 MPa (Variable thermal properties)**

Figure 6.21 shows the top center temperature variations by time. The system is thermally steady state at the end of each response plot. The behavior is comparable with what presented in section 6.6.1.1.

![Figure 6.21](image)

**Figure. 6.21 Top center temperature by time for a constant heat load of 50 mW at 2 MPa (Variable thermal properties)**

Sharp changes appear in the temperature distribution along the beam leading to sharp changes in the deflected shapes at the edges as shown in Figures 6.22 and 6.23.
Figure 6.22 Top center temperature distribution along the beam for a constant heat load of 50 mW at 2 MPa (Variable thermal properties)

Figure 6.23 deflected shape for a constant heat load of 50 mW at 2 MPa (Variable thermal properties)

Figure 6.24 shows the dominant frequencies corresponding to the response shown in Figure 6.20. This shows that the system responds with all the modes for step excitation. The results obtained in section 6.6.1.2 are comparable with the results obtained in section 6.6.1.1.
6.6.1.3. **Constant versus Variable Properties Solver at 1 MPa Air Pressure.** This section presents the thermal and structural response of the beam with the same dimensions as sections 6.6.1.1 and 6.6.1.2 for a heat load of 50 mW added to the top of the beam at time, t=0. The air pressure is reduced to 1 MPa corresponding to the dimensionless damping constant of 0.052. The study was performed for both constant and variable properties solvers. Figure 6.25 shows the response for both cases. Due to a much smaller damping coefficient, it takes a longer time for the response to be damped to a constant value. As a result, four time durations were used to study the behavior.

The constant thermal properties solver is damped to a smaller center displacement due to a smaller thermal expansion coefficient. The settling time is comparable between the constant and variable thermal properties.
Figure 6.25 Response to constant heat load of 50 mW at 1 MPa (a) Constant thermal properties (b) Variable thermal properties

Figure 6.26 shows the top center temperature variations by time for the both solvers. The temperature is not fully steady at the end of the first run as shown in the dashed line.

Figure 6.27 shows the temperature distribution at the last time step of each response along the beam. Other than point “1” which is the last time step of the first response plot, the other temperature distributions are identical. The reason is that the first response plot ends at the very beginning of transition to steady behavior as shown in Figure 6.26.
Figure 6.27 Top center temperature distribution along the beam for a constant heat load of 50 mW at 1 MPa (a) Constant thermal properties (b) Variable thermal properties

Figure 6.28 shows the deflected shapes at the four time points. Each point represents the results at the last time step of each response shown in Figure 6.25. The deflected shape becomes approximately identical at points “3” and “4”. The reason is that the dynamic effects become minimal at these points as shown in Figure 6.25. As previously explained in sections 6.6.1.1 and 6.6.1.2, the deflected shape is a function of temperature distribution. A temperature distribution uniformly distributed along the beam and with a sudden change at the edges leads to large bending moment at the ends and creates sharp displacement slope at the ends, as shown in sections 6.6.1.1 and 6.6.1.2. Figure 6.28 (see a) shows the sharp slope at the ends in the deflected shape for constant properties, however, Figure 6.28 (see b) clearly shows the zero slope at the ends for the deflected shape for variable properties. This trend is observed because the expansion coefficient is parabolic distributed along the beam for the variable properties solver while it is uniform along the beam for constant properties. These results suggest thermal properties as another term playing a significant role in the deflected shape.

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Figure 6.28 deflected shape for a constant heat load of 50 mW at 1 MPa (a) Constant thermal properties (b) Variable thermal properties

Figure 6.29 shows the dominant frequencies in the both cases. Good agreement is obtained between the explicit constant properties solver and the implicit variable properties solver. Both constant and variable solvers indicate the first and second dominant frequencies as exact same values. However, the constant properties solver does not indicate any dominant frequency larger than $4 \times 10^8$ Hz. The implicit solver for constant properties equation is unconditionally stable. As a result, the time step selected for implicit solver is two order of magnitude larger than the time step selected for the variable properties solver to make the computation faster. As a result, the implicit constant properties solver is limited in indicating the large frequencies in the system.

Figure 6.29 Dominant frequencies for a constant heat load of 50 mW at 1 MPa for variable versus constant thermal properties
6.6.1.4. Settling Time. The settling time is investigated for a range of pressures from 0.7 MPa to 5 MPa. As shown in the previous section and Eq. (2.30), damping coefficient is a function of air pressure. Damping coefficient increases as the air pressure increases. This decreases the settling time. Although initially, the heat amplitude does not seem to affect the settling time, a study is performed to investigate the effect of heat amplitude over the velocity of the movement and the settling time of the vibration.

Figure 6.30 shows the settling time variations by pressure. As the pressure decreases, the settling time increases.

![Figure 6.30 Settling time by air pressure](image)

Figure 6.31 shows the settling time by the heat addition to the system for the air pressure of 1 MPa. Although no variation was expected, by increasing the heat addition, the settling time increases.
Figure 6.31 Settling time by heat addition to the system

Figure 6.32 shows the center velocity variation by time for a range of heat addition to the system. Increase in the heat addition increases the center velocity which indirectly affects the damping of the system.

6.6.2 Harmonic Excitation

After performing the mesh independence study as will be explained in section 6.6.2.2, the results are obtained for 100 nodes \( \times \) 11 nodes \( \times \) 9 nodes respectively in the x, y and z directions. \( 10^4 \) number of time steps are selected in each vibration period. The time step is defined as follows:

\[
\Delta t = \frac{1}{10^4} \frac{2\pi}{\omega}. \tag{6.24}
\]
In order to quantify the results, for simplicity another term is defined as the frequency ratio, \( r \). Frequency ratio is the response and excitation frequency, \( \omega \), divided by the natural frequency:

\[
 r = \frac{\omega}{\omega_n}
\]  

(6.25)

where \( \omega_n \) is the natural frequency of the bridge.

Figure 6.33 shows the excitation \( (q''\times10^{10}) \) versus response \( (\nu(x=L/2,t)) \) variations by time for the heat load amplitude of \( A_h=600 \text{ MW/m}^2 \) and frequency ratio of 2.4. The center displacement \( (\nu(x=L/2,t)) \) is measured in the opposite direction of the z axis as shown in Figure 2.1 for the heat added to the top of the bridge. The y axis is not quantified since the excitation and response have different units. This Figure shows the both excitation and response changes by time with the same frequency equal to \( \omega \). However, there is a lag between the excitation and the response. This lag is called phase delay, \( \varphi \) if it is in degrees or time delay, \( \tau \) if it is in second. The response starts from zero and it takes time until it becomes harmonic. The results also show that it takes a couple of periods until the vibration becomes steadily harmonic.

Figure. 6.33 Response versus excitation \( (A_h=600 \text{ MW/m}^2 \text{ and } r=2.4) \)
The first step to quantify the results is to fit the transient thermo-structural response with a function given as follows:
\[
\delta(t) = \delta_s - \delta_v \cos(\alpha t + \phi),
\]  
(6.26)
where \(\delta_s\) is the steady state displacement, \(\delta_v\) is the vibration displacement, and \(\phi\) is the phase delay between the excitation and the response. In order to obtain a reasonable fit, \(\delta_s\) and \(\delta_v\) must be determined when the response becomes harmonic (steady state).

### 6.6.2.1. Thermal versus Mechanical Excitation

Prior to study of the vibration and steady state displacement variations due to the changes in the heat and the pressure, the response is compared with a spring-damper system to study the thermally excited system versus a mechanically excited system. Although the study targets the pressures lower than atmospheric pressure, getting the solution converged is faster for higher pressures as it will be discussed later. The results were obtained using a constant thermal properties solver at 1 MPa.

The phase delay between the response and the mechanical excitation for forced vibration of a single degree-of freedom mass-spring-damper is given by (Kelly, 2012):
\[
\phi = \tan^{-1}\left(\frac{2\xi r}{1 - r^2}\right),
\]  
(6.27)
where \(\xi\) is the damping coefficient and \(r\) is the frequency ratio as shown in Eqs (6.16) and (6.25).

Figure 6.34 shows phase delay variations by the frequency ratio, for the thermo-structural simulation for total heat amplitude \(A_h\) of 600 MW/m\(^2\) and the phase delay in the mechanical excitation in a mass-spring-damper system (Eq. (6.27)). The thermo-structural simulation phase delay increases by the frequency. The results also show that thermal actuation returns larger phase delay than the phase delay in the mechanical actuation in the mass-spring-damper system. The reason is when the structure is thermally actuated, an additional delay is created, due to the time that it takes the heat to travel and cause the thermal stresses.
6.6.2.2. **Mesh-Independence.** The model is initially run for $25 \times 11 \times 9$ nodes in full model for a fixed time step of 1 micro-sec. The objective is to fix the mesh domain for a fixed time step. After obtaining the fixed domain, the run will be repeated for a range of time steps to obtain the time-step-independent results. Figure 6.35 show the results for various divisions in the x direction. The displacement only tracked at the center of the beam by time ($\nu(x=L/2,t)$).

The results show that the mesh independence is obtained as the number of divisions in x direction is increased to 101. The mesh independency is accurate to the third significant digit for this number of divisions.
Figure 6.36 shows the maximum center displacement (within 2000 nsec) versus the number of divisions in x directions. The results totally approach the asymptote value, which shows mesh-independent results are obtained.

![Figure 6.36 Maximum center displacement versus number of divisions in x direction](image)

**6.6.2.3. Response Variation by Heat.** Chapter 2 showed steady state center displacement variations by total heat correspond to a linear system. The same study must be performed for the steady state amplitude, $\delta_s$ and the vibration amplitude $\delta_v$. Figure 6.37 shows the vibration amplitude variations by total heat amplitude for frequency ratio of 1 at 100 kPa for both the constant thermal properties solver and the temperature dependent thermal properties solver. The response for constant thermal properties solver corresponds to a linear behavior with total heat variations while the temperature dependent thermal properties solver returns a nonlinear behavior of the response with the heat addition. In general, increasing the total heat amplitude, $A_h$, has more significant effects on increasing the vibration amplitude, $\delta_v$ rather than the steady state amplitude $\delta_s$. The variation between steady state amplitude and heat is not shown because at the pressures lower than atmospheric pressure, this variable is very small in the order of angstroms.
Figure 6.37 Vibration amplitude variations by heat (r=1)

6.6.2.4. Response Variation by Pressure. Decreasing the pressure affects the vibration and steady state amplitudes by decreasing the damping coefficient, $\xi$ (Eqs. (6.14) and (6.16)) and the heat transfer coefficient. It significantly increases the vibration and steady state amplitudes. Figure 6.38 shows the center displacement versus time for four pressures of 1 MPa (see a), 500 kPa (see b), 250 kPa (see c) and 100 kPa (see d). These results are obtained using the constant thermal properties solver at a low heat amplitude of 1 mW where the behavior is still linear. As it shown in Figure 6.38 (see d), as the pressures drops to the atmospheric pressure the convergence time becomes significantly higher.

Figure 6.39 shows the amplitudes variations by pressure for total heat amplitude of 50 mW. The higher rate of heat addition requires using the explicit temperature dependent thermal properties solver. The vibration amplitude decrease by increasing the pressure. The rate of decrease is significantly lower for the steady state amplitude, $\delta_s$. As previously explained in section 6.6.2.3, steady state displacement is very small, in the order of an angstrom.
As shown in Figure 6.38, obtaining the steady harmonic response becomes challenging as the pressure decreases. Although the steady harmonic response was not obtained for pressures
below 70 kPa, the first 11 cycles as shown in Figure 6.40 (see a and b) show as the pressure decreases below 2.5 kPa the steady and vibration amplitudes remain unchanged. It is the point where heat transfer does not affect the response of the structure.

6.6.2.5. Non-Resonant Response. As the frequency changes to non-resonant frequencies, the convergence time significantly increases. Figure 6.41 shows the center displacement variations by time at frequency ratio of 1.2 and air pressure of 100 kPa. The response behavior shows various frequencies other that the excitation frequency at the beginning. However, after 6000 nsec, the response is damped to only one frequency which is the excitation frequency.
In order to study the frequencies in the system, a Fast Fourier Transform (FFT) method implemented in Matlab is applied to the response. In Figure 6.42 (see a) the FFT is applied to the response in the entire time domain. Two main frequencies are observed: the natural frequency and the excitation frequency.

![Graph of frequency response](image)

(a) Dominant amplitudes by the frequency \(r=1.2, p=100 \text{ kPa}\): (a) Dominant frequencies for the entire data (b) Dominant frequencies after 6000 nsec

If FFT is only applied to the response after 6000 nsec as shown in Figure 6.42 (see b), the only dominant frequency is the excitation frequency. This plot shows the response converges to the excitation frequency after 6000 nsec.

In order to study the amplitudes and phase delay variations by the frequency ratio, a range of non-resonant simulations were performed at 100 kPa using the implicit constant thermal properties solver at 1 mW heat amplitude. The simulations were run up to 7000 to 8000 nsec to ensure the steady harmonic behavior. Figure 6.43 shows the phase delay variations by the frequency ratio. The phase delay variations occurs in a narrow range of frequency ratio between 0.98 and 1.1. Outside of this narrow domain the phase delay is constant either equal to zero \((r<0.98)\) or \(\pi (r>1.1)\). This behavior corresponds to that of forced harmonic vibration for small damping coefficients (Thomson, 1993).
Figure 6.43 Phase delay variations by frequency ratio

Figure 6.44 shows the amplitudes variations by the frequency ratio (see a). The amplitudes are non-dimensionalized using Eq. (3.16).

\[ \delta^* = \frac{\delta k}{q^* \alpha L^2} \]  \hspace{1cm} (3.16)

Non-dimensionalized vibration amplitude, \( \delta_v^* \) is calculated using Eq. (6.28):

\[ \delta_v^* = \frac{\delta_v k}{q^* \alpha L^2} \]  \hspace{1cm} (6.28)

Non-dimensionalized steady state amplitude, \( \delta_s^* \) is calculated using Eq. (6.29):

\[ \delta_s^* = \frac{\delta_s k}{q^* \alpha L^2} \]  \hspace{1cm} (6.29)

The non-dimensionalized amplitudes are shown in Figure 6.44 (see b). The steady state amplitude does not show significant variations by the frequency ratio while the vibration amplitude shows significant variation in the domain between frequency ratios of 0.9 and 1.1. The maximum vibration amplitude falls between 1.008 and 1.02. Comparing with forced unbalanced harmonic vibration results the peak of the amplitude is slightly larger than one for small damping coefficients (Thomson, 1993).
Figure 6.44 Amplitudes variations by the frequency ratio (a) dimensional results (b) Non-dimensional results

Nyquist diagram for non-resonant simulations at 100 kPa is shown in Figure 6.45 for non-dimensional vibration amplitude.
6.7 Conclusion

The thermo-structural simulation of a thermally actuated silicon nano-bridge by a harmonic heat flux shows that the phase delay in a thermally actuated structure is larger than the phase delay in a mechanically actuated mass-spring damper for the same damping coefficient.

The results for frequency ratio 1 where the response frequency is equal to the natural frequency show that the steady state amplitude and the vibration amplitude decrease by increasing the pressure due to an increase in the damping coefficient. The rate of decrease is significantly higher for the vibration amplitude, $\delta_v$. This is due to the combination of increasing heat transfer coefficient, and increased damping, as the pressure increases.

The implicit constant thermal properties solver shows the amplitudes variations by the heat amplitude corresponds to a linear system, however, the explicit temperature dependent solver shows that the constant thermal properties assumption is limited to low heat amplitudes under 1 mW. For higher heat amplitudes the behavior becomes nonlinear.

Non-resonant simulations show phase delay, Bode and Nyquist diagrams are in good agreement with that of forced unbalanced harmonic vibration results. Future work will use this simulation method to determine the control parameter for thermo-structural vibration systems.
CHAPTER 7: SUMMARY AND DISCUSSION

Thermal positioning, buckling and thermal actuation in micro- and nano-electro-mechanical structures are simulated. A three-dimensional bridge with pinned-pinned and fixed-fixed (doubly-clamped) boundary conditions is used as the micro- and nano-structures. The thermo-structural equations corresponding to thermal positioning and thermal actuation are derived and numerically solved using an implicit Finite Difference method implemented in Matlab for the steady state and C++ for the transient study. When the constant thermal properties are changed to temperature dependent thermal properties, an explicit approach is used to solve the transient thermo-structural equation.

7.1 Thermal Positioning

In order to study the thermal positioning of a micro- and nano-bridge, a constant time-independent heat flux is added to the top of the pinned-pinned bridge. The response is the thermally steady state center displacement of the bridge. The system of equations are solved numerically using an implicit Finite Difference scheme implemented in Matlab.

The results are obtained over a range of dimensions (micro-scale to nano-scale), materials (silicon, silicon carbide and CVD diamond), ambient heat transfer conditions (free molecular and continuum approaches), and a range of heat loads. The results are non-dimensionalized to provide insight into thermal positioning across a range of structure length scales and material properties. The results show that the steady state thermal displacement of the system is a function of the geometry. As the ratio of the width to the length of the bridge decreases for constant widths, the value of the displacement increases. As the dimensions of a geometry change by a constant factor, the dimensionless displacement versus the Biot number collapse in all cases for the same material property (Maghsoudi and Martin, 2012a).
The displacement behavior is also a function of pressure, material properties, and constant heat flux in free molecular model, while this value is independent of pressure in the continuum model because the heat transfer coefficient is pressure-dependent in the free molecular case. The displacement increases as the constant heat flux at the top surface increases. The displacement variations by total heat added to the structure in this model corresponds to that of a linear system. Overall, ambient cooling strongly influences the displacement of thermally-positioned nano-scale devices. The Biot number determines the dimensionless displacement of the bridge.

The individual atoms of the cantilever are vibrating, causing a very small, but quantifiable displacement which is defined as thermal noise (Stowe et al., 1997; Datskos et al., 2003). The thermal displacement which is a function of the average temperature of the structure and the mechanical stiffness of the system is the representative of the thermal noise. The Displacement Ratio (DR) is defined as the center displacement, created by thermal stresses, divided by the thermal displacement. Thermal noise analysis and the displacement variations by pressure suggest silicon carbide as the most appropriate material to fabricate nano-devices where positioning accuracy is a design requirement. This shows the displacements of the order of angstrom for an average heat load and thermal noises of tens of the order of the magnitude.

The presented data are worthwhile since the measurements are difficult commonly in micro- and nano-system design. Furthermore, the computational results in thermal positioning are verified by analytical rectangular cross section fin results. Also, the results are qualitatively compared with the previous experimental results.

The methods developed in the thermal positioning study are applied to simulate two nano-micro-scale devices: an existing thermally actuated micro-switch configuration, and a new nano-mechanical memory configuration.
7.1.1 Thermal Micro-Switch

In 2001, Blondy et al. fabricated a thermally actuated silicon nitride micro-switch bridge. The heat was added to the sides of the top surface of the switch. Their experimental measurements showed that the switch had low actuation voltages (Blondy et al., 2001).

In order to obtain the closing and opening times and opening time lag, the dynamic structural equation including the acceleration and inertia effects must be simulated. The dynamic structural equation is not solved in this work. Instead, steady state structural equation is simulated to obtain thermally steady state center displacement. As a result, thermal positioning can only investigate the power consumption and thermal efficiency in the thermal micro-switch.

The study is performed on a switch with a length of 250 microns. Three heating configurations are used: distributed heating at the top surface, concentrated heating at the center of the top surface, and concentrated heating at the sides of the top surface. The study is performed for two materials: silicon and silicon-nitride. The results show that distributed-heating configuration and center-heating configuration show the closed switch operates more efficiently than the open switch. This will lead to a thermal lag in opening the switch.

For a specific steady state center displacement for distributed-heating configuration, closed switch requires less heat at the top than open switch. Open silicon-bridge shows the overall efficiency coefficient of 11.8 nm/W while closed silicon-bridge shows the overall efficiency coefficient of 15.9 nm/W. These values increase to 66.1 nm/W, and 89.1 nm/W for silicon-nitride-bridge.

The contact length variations have negligible effects on the steady state center displacement of the bridge. Increasing the contact length to twice and three times of the initial contact length results in the maximum difference of less than 3 nanometer in the steady state center displacement. The contact temperature increase will decrease the temperature gradient in the z direction leading
to a lower efficiency. The lower temperature gradient is observed at the contact temperature of 305 K. However, the efficiency decrease is 1.5% for contact temperature increase from 290 K to 305 K.

Heat addition to the center of the top surface of the bridge is the most efficient way to obtain a larger center displacement per unit heat addition. It is more thermally efficient than adding concentrated heat to the sides of the top surface by a factor of 17 in closed switch and 8.8 in open switch. In center-heating and side-heating configurations the switch efficiency coefficient is a function of heating length. As long as the heating length affects the temperature gradient in the z direction, it can change the efficiency coefficient.

For the center-heating configuration, the efficiency increases as the heating length increases up to 50 microns. Any increase in the heating length over 50 microns leads to a decrease in the switch efficiency. For both open and closed switches, 50 microns returns the maximum pick of the efficiency coefficient in center-heating configuration. The efficiency decays by increasing the heating length further than 120 microns and eventually it becomes equal to the efficiency coefficient of the distributed heat configuration.

The side heating configuration’s efficiency coefficient increases linearly by the heating length. The efficiency difference between the open and closed switch is negligible for the heating lengths up to 120 micron. The efficiency is expected to merge with the distributed heat’s efficiency coefficient as the heating length increases up to 250 microns.

These results can be applied to the existing thermal micro-switches, such as those designed by Blondy to improve the efficiency. Selectively applying the heat to the top center of the switch instead of the sides will improve the efficiency by a factor of 17 in closed switch and 8.8 in open switch.
7.1.2 Thermal Buckling Nano-memory

The two technologies of buckling beam and thermal excitation are used to design a storage nano-memory. A unit bridge of an array of buckling-beam memory (a thermally actuated nano-bridge) is simulated using the same Finite Difference scheme used for thermal positioning in chapter 2. Power requirements for thermal actuation, optimal geometry, and write time of the device for various materials are investigated.

The results show that the energy required for writing data per bit is in the order of 1 nJ which shows low power consumption of the device. Data storage density is a trade-off. In order to balance these constraints, a length of 20 microns and the smallest possible thickness to fabricate, is suggested. This design suggests a memory density in the order of $10^6$ bits/cm$^2$ and $10^{11}$ bits/cm$^3$ which are acceptable in comparison with the current memory devices and can be improved by decreasing the width and the thickness of the beam.

Decreasing the thickness and the width is desired for both energy consumption and buckling time. However, decreasing the length has reverse effects. The buckling time changes inversely with the total heating rate and the length of the beam. The simulation results show that the write time of less than 10 nsec/bit is achievable (100 MB/sec). Because this technology allows reading and writing in parallel, the writing process can be accelerated using multiple reading/writing heads.

The study was performed for various materials. The results show that PMMA, parylene, and kapton bits consume the least power and buckle faster than silicon and silicon carbide bits.

This type of storage memory can be applied to high radiation and electromagnetic environments encountered in space exploration. The radiation constraint is the most difficult for these systems, and is the largest barrier to qualification of memory systems for spaceflight (Nguyen et al., 1999; Scheick et al., 2000). In the highly radioactive environment of space, high energy protons and electrons may strike the structure. These particles can be a result of solar events or the
planetary environment (Fortescue et al., 2003). This can cause the single event upset for conventional semi-conductor devices. Current missions to the Jovian system use a radiation locker for all the electronics to avoid scrambling the data in conventional memories. Therefore, the system must be designed not to buckle after high-energy collisions.

The results for high energy particles collision show that electron collision causes buckling in the PMMA, parylene, and kapton bits. High energy particle collision will not lead to undesired buckling in the silicon and silicon carbide memory bits. The heat due to the collision dissipates in less than 10 nsec. As a result, either silicon or silicon carbide is the most appropriate material to fabricate the device for Jovian moon or other extreme environments. However, PMMA, parylene, and kapton are more appropriate alternatives for other missions where radiation environment is not extreme.

The results obtained using the simulations in chapter 5 including all the simplifications report the suggested memory is a radiation protected memory storage with an acceptable writing time, power consumption and data storage density. However, there is no doubt that the simulations can be improved by using the temperature dependent thermal properties solver for the heat conduction equation, adding other materials to the silicon layer and improving the buckling structural solver using a more sophisticated buckling formulation. Fabrication and providing the preliminary test data can significantly improve the simulations.

7.2 Thermal Actuation

Thermal actuation which is applying sinusoidal heating leading to vibration in the bridge is simulated for the nano-bridge structures. The heat addition is harmonic and time-dependent. Silicon is the selected material for the study and free molecular approach is used to define the heat transfer coefficient.
The structural equation is re-derived to take into account the acceleration and inertia effects to study the dynamic behavior of the system. An implicit Finite Difference scheme implemented in C++ was used to solve the coupled thermo-structural equations at each time step. While an explicit scheme was used for temperature dependent thermal properties. The response, the center displacement is tracked by time and decomposed to steady state amplitude and the vibration amplitude when the harmonic solution was achieved.

The results obtained with the mesh-independence accuracy of three significant digits show that the phase delay between the excitation and the response in a thermally actuated structure is larger than the phase delay in a mechanically actuated mass-spring damper for the same damping coefficient.

The results were obtained for under atmospheric pressure. Decreasing the pressure will decrease the damping coefficient, $\xi$ and heat transfer coefficient, $h$ leading to an increase in the both amplitudes. The rate of increase is significantly higher for the vibration amplitude. As the pressure decreases below 2.5 kPa the vibration amplitude remains unchanged.

The non-resonant results show that the steady state amplitude remains constant as the frequency changes. However, at low damping coefficients, the vibration amplitude increases by the frequency ratio $r$ until it becomes slightly larger than 1 (1.008 at 100 kPa). Increasing the frequency ratio larger than that leads to a decrease in vibration amplitude.

The thermal actuation simulation can be applied to study the thermal micro-switch dynamic behavior. In order to study the dynamic behavior of the thermal micro-switch, a correct contact model as well as viscous damping coefficient must be added to the simulation. Previous researchers showed that the viscous damping coefficient is a function of the gap size in electrostatically actuated MEMS switches (Snow and Bajaj, 2011; Guo and Alexeenko, 2009; Bao and Yang 2007). However, none of these models guarantee to propose the perfect viscous damping
coefficient. Adding the contact and viscous damping coefficient will provide the simulation of the closing and the opening moment in a thermal switch. The moment of the detachment of the switch from the contact requires more investigation. Overall, the thermal actuation simulation provides sufficient information to begin the study of the micro-switch dynamic behavior as a future research scope.

### 7.3 Future Projects

In summary the following projects can be defined in the continuation of the current study:

1. Improvement of the unsteady thermo-structural solver implemented in chapter 5 and applying it to control simulations.

2. Adding the contact and viscous damping coefficient to the unsteady thermo-structural solver implemented in chapter 5 to simulate the closing and the opening moment in a thermal switch.

3. Fabrication and testing a single bit of buckling beam memory using the provided data in chapter 4 and continuation of the simulation using a more sophisticated buckling structural simulation.
REFERENCES


VITA

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