Analysis of effective mechanical properties of thin films used in microelectromechanical systems

Ajay Pasupuleti
ANALYSIS OF EFFECTIVE MECHANICAL PROPERTIES
OF THIN FILMS USED IN
MICROELECTROMECANICAL SYSTEMS

by

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Analysis of Effective Mechanical Properties of Thin Films used in MicroElectroMechanical Systems

By

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ABSTRACT

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This research aims at analyzing the effective mechanical properties of thin film materials that are used in MEMS. Using the effective mechanical properties, reliable simulations of new or slightly altered designs can be performed successfully. The main reason for investigating effective material properties of MEMS devices is that the existing techniques can not provide consistent prediction of the mechanical properties without time-consuming and costly physical prototyping if the device or the fabrication recipe is slightly altered. To achieve this goal, two approaches were investigated: soft computing and analytical. In the soft computing approach, the effective material properties are empirically modeled and estimated based on experimental data and the relationships between the parameters affecting the mechanical properties of devices are discovered. In this approach, 2D-search, Micro Genetic Algorithms, Neural networks, and Radial Basis Functions Networks were explored for the search of the effective material properties of the thin films with the help of a Finite Element Analysis (FEA) and modeling the mechanical behavior such that the effective material properties can be estimated for a new design. In the analytical approach, the physical behavior of the thin films is modeled analytically using standard elastic theories such as Stoney’s formulae.

As a case study, bilayer cantilevers of various dimensions were fabricated for extracting the effective Young’s modulus of thin film materials: Aluminum, TetraEthylOrthoSilicate (TEOS)-based SiO₂, and Polyimide. In addition, a Matlab® graphical user interface (GUI), STEAM, is developed which interfaces with Ansys®. In STEAM, a fuzzy confidence factor is also developed to validate the reliability of the estimates based on factors such as facility and recipe-dependent variables. The results obtained from both approaches generated comparable effective material properties which are in accord with the experimental measurements. The results show that effective material properties of thin films can be estimated so that reliable MEMS devices can be designed without timely and costly physical prototyping.
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Chapter 1: Introduction

Miniaturization has been one of the most important technology trends over the last decade. Over the years, the sizes of sensors, processing electronics, and actuators have been reduced from centimeters to millimeters and very high component densities have been achieved [1-7]. These micro-components when integrated form Micro Electro Mechanical Systems (MEMS) devices that have complex 3-D shapes and sizes but are small in size and weight, and consume very low power. This technology offers great potential for implementing very powerful miniaturized devices for sensing and acting upon the physical world. These micro-components can be integrated to implement useful devices for a wide range of areas such as microelectronics, electromagnetic, optical, and biological technologies. Table 1 illustrates the growth in the MEMS market from 1995 to 2005 [1]. This advancement was possible primarily due to the rapid growth and development in the engineering sciences especially in the area of thin films that range from a few angstroms to a few microns in thickness [5-7].

Due to the widespread applications of the MEMS devices, recent emphasis has been on improving device behavior models for performance enhancement and long-term reliability [5-8]. In order to achieve this goal it is necessary to understand the mechanical properties of thin films. However, mechanical properties of thin films are not extensively available and extrapolating these properties from the bulk parameters has been determined to be very unreliable [9-11]. Due to this limitation, Computer Aided Design (CAD) of MEMS devices is still in its infancy and current day MEMS devices are often realized by physical prototyping, which is an expensive and time consuming process. As
a result, the focus of the recent research has been on the development of material properties estimation techniques that can be utilized in CAD tools for MEMS [12]. This is because software tools, when sufficiently precise and computationally effective can be commercially advantageous in shortening the design cycle and thus could prove to be cost effective.

Table 1.1: Bryzek’s MEMS market forecast [1]

<table>
<thead>
<tr>
<th>Year</th>
<th>1995</th>
<th>2005</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure sensors</td>
<td>$1.0B</td>
<td>$2.5B</td>
</tr>
<tr>
<td>Inertial sensors</td>
<td>$0.4B</td>
<td>$0.8B</td>
</tr>
<tr>
<td>Fluidic controls</td>
<td>$0.01B</td>
<td>$0.1B</td>
</tr>
<tr>
<td>Data storage</td>
<td>$0.0B</td>
<td>$1.0B</td>
</tr>
<tr>
<td>Displays</td>
<td>$0.0B</td>
<td>$1.0B</td>
</tr>
<tr>
<td>Biochips</td>
<td>$0.0B</td>
<td>$0.2B</td>
</tr>
<tr>
<td>Communication</td>
<td>$0.01B</td>
<td>$1.0B</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>$0.03B</td>
<td>$0.1B</td>
</tr>
<tr>
<td><strong>Total MEMS</strong></td>
<td><strong>$1.45B</strong></td>
<td><strong>$6.7B</strong></td>
</tr>
<tr>
<td><strong>Total non-sensing MEMS</strong></td>
<td><strong>$0.05B</strong></td>
<td><strong>$3.4B</strong></td>
</tr>
</tbody>
</table>

Consequently, this research proposes a novel methodology for estimating the material properties of thin films that are utilized in MEMS transducers. A software framework is also proposed that could be used for static and dynamic analysis for MEMS actuators. The proposed approach is very similar to the behavior models that were incorporated in the SPICE® tools that were developed for the microelectronics industry [13]. One can clearly associate the success and the current state of the electronic industry to the models that can predict the behavior of the electronic components to a great accuracy which results in high reliability and efficiency. Likewise, in this research
empirical models will be developed that are based on experimental data and theoretical analysis. Models designed in this process are foreseen to be essential tools for MEMS designers as they would relate the loading parameters, material properties, and geometry of the microstructures with their performance characteristics. Modeling software such as the one proposed enables designers to prototype and/or simulate the designs accurately before fabrication. As a result, this process aids in accelerating the design and development process of MEMS devices thus making them cost effective. Due to these advantages, the models developed in this research would prove to be very useful for MEMS researchers as well as the industry in developing accurate MEMS devices.

The following paragraphs describe the chapters of this dissertation. **Chapter 2** contains a literature review on CAD for MEMS covering the various components of the mechanical behavior models as well as the material property databases used in the existing software packages. This provides a background to the limitations of the existing methodologies and lays the foundation for empirical estimation techniques studied in this dissertation.

**Chapter 3** describes the proposed methodology along with the software implementation that is called *Simulation Tool based on Empirical Analysis for MEMS* (STEAM). The highlights of this software tool are the Matlab®- Ansys® interface, integrated soft computing techniques and fuzzy logic based confidence factor.

**Chapter 4** illustrates the working of the proposed methodology with a case study. Mechanical behaviors of aluminum, SiO$_2$, and polyimide thin films were analyzed using micromachined bilayer cantilevers. This analysis was performed using two techniques that have different fundamental assumptions. This chapter illustrates the working of these
two techniques. In addition to this, the effect of change in recipe parameters on the material properties is discussed by studying the mechanical properties of aluminum thin films that are deposited under different process conditions.

Chapter 5 describes the fabrication and simulation results pertaining to the bilayer cantilevers. This chapter consists of four main subsections. The first section deals with the fabrication results of the bilayer cantilevers. In the second section a comparison of the deflections obtained by the bulk value and the experimental values is shown. This section also illustrates the working of the soft computing approach as well as the design and fabrication of a novel MEMS-based micro mirror that was conceived to test the accuracy of the effective material properties generated by the proposed methodology. In the third section results pertaining to the analytical technique are illustrated. Finally, the working of the proposed fuzzy confidence factor is shown in the last section.

Chapter 6 describes the conclusions as well as illustrates the possible extensions to the proposed methodology.
Chapter 2: Background

Commercial success of most present-day MEMS devices such as accelerometers and pressure sensors is attributed to the reliable and reproducible models that were developed by extensive physical prototyping [5, 12]. This process involves tedious, cost ineffective and time-consuming iterations in the device designs, material selections, and the fabrication runs [5, 12]. Although some of these parameters are very specific to the MEMS device under consideration, the developed models were very specific and non-portable [5]. As a result, the rapid prototyping of new devices was not possible which in turn effected the commercialization of MEMS technology [5-8, 12]. Due to this limitation, recent years have seen the development of several simulation and CAD tools that can predict the performance of the MEMS devices.

This chapter describes the literature survey on CAD for MEMS as well as the general architecture adopted by the existing software packages. While describing these software packages, special emphasis is placed on the material property generation modules because the performance of the MEMS devices are greatly dependent upon the material properties [14-17]. This discussion will lead to the identification of the limitations of the existing techniques (MEMS software packages) and the problem statement for this research.

This chapter is organized as follows. Section 2.1 describes the general architecture of the MEMS computer aided design. In Section 2.2, the material property database used in the existing software packages is analyzed. This is followed by a literature survey of the state of the art modeling techniques in Section 2.3. Finally, in
Section 2.4 the limitations of the existing techniques are illustrated along with the problem statement of this research.

2.1 General architecture

Computer aided design (CAD) of MEMS devices is comprised of several descriptive levels that are commonly executed in a sequential order. These levels can be grouped into three main categories that are geometry, fabrication, and modeling of the MEMS device. Unlike the microelectronic industry which deals with primarily two-dimensional circuits (products) that are fabrication independent, MEMS technology is often three dimensional and the fabrication process must be custom designed for a specific product [12]. As a result, in addition to three dimensional simulation and visualization levels, MEMS simulation tools must consist of the fabrication process simulation that is specific to the device under consideration. Information from these levels can then be used for modeling the performance of the MEMS device. Figure 2.1 presents a functional sequence of the various modules in the simulation of Microsystems [12].

In this architecture, information pertaining to the geometry of the MEMS device is obtained to describe the layout and device topography. This information is fed into the process simulator module and possible fabrication sequence is computed. The obtained structural information is then sent to the device simulator module along with the material properties of all the materials involved in the device fabrication. In the device simulator, appropriate physical models that best describe the MEMS device are selected to perform numerical analysis.
Depending on the problem at hand, steady-state or transient analysis is performed in the appropriate energy domain (structural, electrical, or coupled analysis) and performance parameters such as input-output characteristics and response functions are quantified and analyzed [12].

![Diagram of General architecture of CAD tools for MEMS](image)

**Figure 2.1: General architecture of CAD tools for MEMS [12]**

The architecture shown in Figure 2.1 has been the foundation for various software tools that were developed for MEMS. Table 2.1 illustrates some of the most commonly used software packages, some of which are commercially available.
In all the software packages listed in Table 2.1 material property generation and utilization and the modeling techniques used for analysis are of primary concern.

Table 2.1: Comparison between the various software packages developed for MEMS

<table>
<thead>
<tr>
<th>Software Package</th>
<th>Geometry</th>
<th>Fabrication</th>
<th>Modeling</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D SURFILER [18]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>GEODISC [19]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>SOLIDS [20]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>AUTOMEMS [21]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>MEMSCAP [22]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>INTELLISUITE [23]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>Sugar [24]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>MEMCAD [25]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>CAEMEMS [26]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
<tr>
<td>MOSCITO [27]</td>
<td>♦</td>
<td>♦</td>
<td>♦</td>
</tr>
</tbody>
</table>

These modules are described in the following sections.

2.2 Material property database

Material properties used in these simulators were based on detailed fabrication process steps or the bulk values reported in the literature [21-27]. Figure 2.2 illustrates the schematic for material property database developed as a stand-alone object-oriented database for the MEMCAD software package [28]. Although this database is very
specific to MEMCAD, it captures the essence of the material property generation and utilization by all the software packages listed in Table 2.1.

![Diagram of material property database]

**Figure 2.2: Schematic of the material property database used in MEMCAD [28]**

In this technique, data pertaining to the material properties for each material (e.g. SiO₂) are collected and organized based on the material type (e.g. amorphous), class of process used (e.g. LPCVD), and specific process details (e.g. temperature) [28]. This information is obtained from the experimental data, from the literature, or other fabrication facilities. Using nonlinear regression techniques, algebraic equations are computed to relate the process parameters and material properties. A query to the database results in either a default value (if experimental data are not available) or an interpolated value that is in the experimental range defined by the user. This information is then utilized by the CAD tool for modeling the MEMS devices [28].

The following section illustrates the mechanical behavior modeling techniques described in the literature.
2.3 Modeling techniques

In the literature, various techniques are proposed for modeling the mechanical behavior of MEMS devices. These techniques can be broadly classified into two categories: analytical modeling and numerical modeling [29].

2.3.1 Analytical modeling

A behavioral model developed using analytical techniques is a well-characterized and widely used technique [29-33]. A schematic of this approach is illustrated in Figure 2.3, where $q$ is the distributed load on the beam, $E$ is the elastic modulus, $L$ and $t$ are the length and thickness of the beam, respectively. In this technique, microsystems are expressed in terms of physical phenomena and their mathematical descriptions. By applying boundary conditions to the partial differential equations, the mathematical equations are obtained which could be solved either exactly or approximately.

![Figure 2.3: Schematic of the analytical behavior modeling [29]](image)

Recent theoretical studies involve the use of testing equipment that is capable of applying loads in the order of micro and nano Newtons [30]. These techniques require a
complicated and special experimental setup [31]. An example of such a technique is load-deflection tests using electrostatic voltage and pressure loads [31]. Other experimental methods involve measuring load-deflection data pertaining to force loads applied by atomic force microscopy (AFM) [30], surface profilometer [32], and nanoindentor [33]. In these techniques the mechanical properties are obtained by the compilation of the deflection data, beam theory, and geometry of the structures. However, in all these techniques, the effect of residual stresses in the beams has been ignored. As a result, the mechanical properties computed cannot model the initial deflection of beams produced by the residual stresses.

Another indirect analytical method devised for determining the mechanical properties of thin films involves deposition of a material of unknown properties on a material of known properties resulting in an initial deflection without any external load [31]. The radius of curvature of the produced deflection is computed using scanning electron microscopy (SEM). The mechanical properties of the unknown material are then derived by substitution of the computed values in the classical residual stress equations [34]. In summary, this approach is efficient if the microstructure can be idealized to its corresponding macrostructures with respect to their boundary conditions.

### 2.3.2 Numerical modeling approach

This technique utilizes powerful tools such as finite element analysis (FEA) for solving the mathematical representation of the given microsystem [29]. Figure 2.4 illustrates the schematic of this approach.
The FEA tools reduce the partial differential equations that are derived from the physical phenomena to algebraic equations which can be simplified numerically. Behavior models are then extracted from these solutions.

\[
\delta = f(q, E, L, t)
\]

**Figure 2.4: Schematic of the numerical approach [29]**

Using this technique, researchers have modeled many complex structures with real boundary conditions [29]. Models developed using this technique were found to have good correlation with results obtained from the FEA tools [29]. However, this technique is limited by the analytical tool used and does not account for actual fabrication dependent parameters such as the effect of residual stress or stress gradient. This limitation may result in a discrepancy between the actual behavior (fabricated values) and the predicted behavior.
In summary the existing techniques are deficient in reliable modeling of MEMS devices. The following section describes their limitations thus the paving way for the problem statement of this dissertation.

2.4 Problem statement

Thin films of glass, silicon, nitrides, and metals find their applications in MEMS as structural materials. Existing software tools model the material properties of these thin films based only on fabrication process parameters and bulk material properties. Recent analysis of thin film materials revealed that the material properties are significantly different from the bulk values [35, 36]. Although the reason for this variation has not been fully understood yet, it is a well accepted fact that size-effect as well as thin film deposition techniques (such as evaporation and sputtering) play a critical role in the micro-world [10, 35]. These factors greatly influence the material properties of thin films and understanding the mechanical behavior is still at its infancy [35]. It was found that process variables such as substrate temperature, working gas species and their pressures, and the orientation of the deposition surface relative to the direction of coating affect the residual stresses in the material during deposition [10]. This discussion illustrates that apart from the recipe parameters there are other parameters that are very specific to the deposition tool, which influence the material properties. As a result, a material deposited using similar deposition technique in two different fabrication facilities may differ in properties. One can say that material properties of thin films are very much dependent on the tools available in the fabrication plant as well as the ambient conditions specific to the plant. This behavior is pictographically represented in Figure 2.5 using the RIT fabrication facility as an example [37]. This figure illustrates that material properties of
the aluminum thin films used in the analysis of MEMS devices such as cantilever etc. are dependent upon the deposition tool (evaporator or sputter) present in the fabrication facility.

![Diagram of fabrication process](image)

**Figure 2.5: Material property dependency over the fabrication plant**

Hence any generalization of the material properties over the fabrication facilities could result in an inaccurate modeling. Another major limitation in the behavior models mentioned above is that they do not take into account the fabrication results in their model extraction. This is a critical component in the design process because the phenomena that apply at the micro scale are not fully understood [35]. For example, in the case of micromachined cantilevers the support structure that is formed is a function of the etch process used in the fabrication. However, reliable etch models can be obtained by extracting empirical models from experimental data [29]. As a result, analytical models that are developed without experimental input could be inaccurate and unfit for prediction. These disadvantages emphasize the need for CAD tools that utilize more accurate material property estimation techniques. The proposed methodology attempts to solve these problems and is described in the following chapter.
Chapter 3: Software Tool Based on Empirical Analysis of MicroElectroMechanical Systems (STEAM)

Understanding the mechanical properties of micro-scale materials is an essential component in the design and development of MEMS devices. A simple tensile tester can describe most mechanical properties at the macro-scale. However, the geometry of the MEMS device and processing history of the materials used have an enormous impact on mechanical behavior at the micro scale. As a result, this research introduces the concept of “effective parameters” for quantities such as the elastic modulus, which takes into account not only the “pure” elastic modulus of the ideal material, but also modifications in the material behavior arising from small geometries, built-in residual stresses, and other processing effects.

This chapter describes the proposed methodology that can extract empirical models for material properties for various materials as well as the software tool that was developed based on this methodology.

3.1 Methodology

As discussed in Chapter 2, mechanical behavior models for thin film materials are still in their infancy [14, 15, 35]. As a result, this research emphasizes investigating novel methodologies that can generate useful material properties in the micro-scale domain. The proposed technique is based on the empirical analysis of experimental data obtained for a wide range of test samples. The fundamental claim of this technique is that by modeling the mechanical behavior through experimental measurements of
standard test structures, the material properties of thin films can be predicted and be used for analyzing other microstructures with similar dimensions.

The working of the proposed methodology (illustrated in Figure 3.1) is as follows. The first step in this methodology is to identify a test structure that can extract the desired material property. This step is followed by the identification of the physical phenomena and the boundary conditions that define the given test structure.

![Figure 3.1: Schematic of the proposed methodology](image-url)
Using this information, the relationship between the governing factors is obtained and expressed in terms of algebraic equations. These equations are then analyzed to generate closed loop solutions. Due to the complexity involved in the 3D MEMS designs, in many situations such a solution is not readily available. Under such circumstances, the proposed methodology emphasizes finite element analysis of the experimental data. With the careful note of the tool as well as the recipe used for fabrication, experimental results are obtained by fabricating the test structure of various dimensions. Results pertaining to the physical dimensions of the test structure, fabrication induced parameters (i.e. induced stress) and feedback parameters (i.e. deflection) are collected using metrology tools such as the SEM and profilometer [37]. These experimental results are then correlated to the analytical solution or the FEA for a large number of data sets. Empirical models that describe effective material properties for the test structures are generated using generalized data fitting (or modeling) techniques, such as radial basis function networks and neural networks.

The above methodology estimates the mechanical properties of the thin film materials based on the deposition technique which includes the tool as well as the recipe used in the fabrication plant along with the physical dimensions of the microstructure under study. Figure 3.2 illustrates the schematic of the material property estimation (data fitting) procedure.

In Figure 3.2, $X$ represents the dimensions of the MEMS structure; $E$ represents the bulk values of the material properties: $\hat{E}$ represents the estimated values, and $y(d)$ and $y'(d)$ represent the experimental and simulation outputs, respectively.
The material property estimation procedure consists of two phases that are model generation and model utilization. In the model generation phase, empirical models are generated by analyzing the tool response as measured by parameters such as the cantilever deflection for a given set of thin film dimensions and environmental conditions [37].

![Diagram of material property estimation process](image)

**Figure 3.2: Material property estimation process in the proposed technique**

After training, the empirical models in the model utilization phase would be capable of generalizing the tool behavior and hence as a result would be able to predict the output for any given dataset.

The following section describes the various components of the proposed methodology. Section 3.1.1 illustrates the characteristics of an ideal test structure. Section 3.1.2 describes the fabrication and metrology computation issues that need to be
considered during the fabrication of the test structure. Finally, Section 3.1.3 describes empirical model extraction techniques that could be used for the model generation phase.

### 3.1.1 Test structure and their importance

Test structures are those devices that have a predefined input-output relationship which can be accurately characterized [7, 15]. These structures play a vital role in the fabrication of microelectronics components as well as MEMS devices. In the microelectronics industry, these structures are often fabricated along with the device to provide information on process uniformity, repeatability, and device performance [7, 15]. This information is used to calibrate the process variables which in turn improve the yield as well as the reliability of the final devices. However, in MEMS these structures have additional significance. Test structures have been commonly used in MEMS for calibrating the simulation models as well as estimating the material properties of various thin films [7, 15, 34-36]. Due to the lack of proper understanding of the mechanical behavior in the micro-scale domain, empirical models are extracted based on experimental device behavior and the system level description of the device. This limitation resulted in the design of test structures that are very specific to a MEMS device. The disadvantage of such a technique is that the extracted parameters have limited applications and are often restricted to a design space that is very similar to the test structure. Recent efforts are underway in developing test structures that can infer material properties in the micro-scale domain, thereby increasing the design space [14-17]. As a result, ideal test structures for material property estimation are those that are easy to fabricate, free from calibration errors, and operate in fewer number of energy domains. These restrictions on the selection of the test structure are due to the fact that
coupled field analysis in the micro-world is relatively new and underdeveloped [14-17]. Apart from these restrictions, it is desirable to conceive test structures that are easy to fabricate [7, 15]. The following section illustrates the reasons for this need with a description of the common sources of error with complex test structure designs.

3.1.2 Fabrication of the test structure

As described in Chapter 2, fabrication process parameters greatly affect the material properties of the thin films. Some of the fabrication related affects on the mechanical behavior of thin films are recipe parameters, boundary conditions, initial geometric conditions, and metrology computation. These parameters greatly influence the modeling approach. Hence these properties are referred to as fabrication-induced parameters. The following section describes these parameters briefly.

3.1.2.1 Recipe parameters

Fabrication of MEMS devices involves a combination of deposition, patterning and etching processes of thin films. In the literature, it was shown that process parameters have an enormous effect on the material properties of thin films [28]. Researchers found that thin films, which are deposited using the same tool but with different recipes, had different properties [5]. For example, thin films of aluminum deposited via DC sputtering with and without substrate heating had substantially different properties. A detailed discussion on this behavior is given in Chapter 5. This discussion illustrates that effective material properties are very specific to the process.
3.1.2.2 Boundary conditions

Due to the complex interactions between the thin films and the various deposition and etching processes, characterizing the supports for the microstructure is multifaceted [29]. For example, cantilever structures fabricated by etching silicon using a wet process have a different anchor structure than those cantilevers released in a dry etch process [29]. This variation in the anchor structure can result in a noticeable change in the constraints imposed on the modeling of mechanical behavior of the thin films [29]. Depending upon the complexity of the test structures, these constraints can quickly add up to make the finite element analysis formidably challenging. As a result, ease of fabrication of the test structure is highly desired and care should be taken in developing the fabrication processes.

3.1.2.3 Initial geometry condition

During the deposition process, residual stresses are introduced into the thin films which could affect the initial geometry of the microstructures [34]. For example in the case of cantilevers, the residual stresses in the thin films result in a static self-deformed, out-of-plane deflection (illustrated in Chapter 5). This behavior has to be considered during the modeling, otherwise significant departures are observed between the experimental and simulation results.

3.1.2.4 Metrology computation

Depending upon the material property under investigation, geometry of the test structure as well as fabrication-induced parameters play a vital role in the computation of effective material properties. These parameters are often computed using various
metrology tools such as surface scan profilometer, optical profilometer, scanning electron microscope as well as optical microscope [37]. Although these tools are known for their performance, accurate metrology is restricted to important structural features depending upon the test structure design [15]. As a result, metrology tools introduce certain amount of uncertainty in effective values.

The next step in the proposed methodology is to extract empirical models from the available experimental data. This process is illustrated in the following section.

3.1.3 Empirical model extraction

As discussed in previous sections, due to the lack of proper understanding of the physical phenomena that relate the device dimensions and process dependent parameters, developing analytical techniques may be a complex task. For example, the various factors that influence the Young’s Modulus of bilayer cantilevers are the dimensions of the beam and the initial stress induced into the thin films (discussed in Chapter 4). As the effect of these parameters is highly non-linear and difficult to compute [34], effective models can be developed by empirical modeling techniques that are based on experimental measurements. In the literature various techniques have been reported for predicting as well as learning the behavior of complex relationships between the design variables [38-40]. Among the various factors that affect the choice of the algorithms is the amount of training data available and the number of design variables that govern the mechanical behavior of the system.

The available algorithms can be broadly classified as parametric and non-parametric algorithms. In parametric methods, the behavior that is being predicted is assumed to obey some distribution that is known and can be described mathematically
(e.g. Gaussian). Examples that describe this algorithm are maximum likelihood estimation, Bayesian estimation, and standard regression techniques [40]. The main disadvantage with parametric methods is that they assume that the sample space describes the whole space. In most cases this assumption may not be valid.

This disadvantage is overcome in the non-parametric methods where the primary assumption is that similar inputs have similar outputs [40]. As a result, the emphasis is on modeling the similarities in the data. Also in this technique available data is classified into training set and test set. By doing so, the performance of the learning algorithm can be easily monitored. Most learning algorithms such as radial basis function networks, neural networks, and support vector machines fall in this category.

Apart from the above estimation procedures, there is a need for developing search techniques that are fast and efficient. These algorithms are needed especially for estimating the effective elastic modulus of the thin films that matches the experimental and simulation results. In the literature, several techniques have been proposed to solve this problem [40]. Among them gradient descent, genetic algorithm, and K-means clustering algorithm-based search techniques have been most widely used [38, 40]. The above discussion clearly illustrates the need for various search and learning algorithms along with finite element analysis for estimating the effective material properties.

The following section describes the software implementation of the proposed methodology which is called STEAM.

### 3.2 Software implementation

The proposed software tool based on empirical analysis (STEAM) was developed using the above described methodology (Section 3.1). Figure 3.3 illustrates the block
The tool has five main components which are model geometry generation, estimation of the material properties, analysis (steady state or transient), result verification, and optimization.

![Diagram of the proposed software tool](image)

**Figure 3.3: Schematic of the proposed software tool**

The algorithms for the five components were developed in Matlab® and Ansys®. The working of the proposed tool is as follows. The first step in the tool utilization process is to generate material properties models for various materials that shall be utilized in the fabrication plant. After the material models are generated, the inputs to the simulation tool are the fabrication process details and the dimensions of the MEMS structure under consideration. Using this information the tool computes the material properties of the MEMS structure. Steady state or transient analysis can then be performed by passing variables and results back and forth between Matlab® and Ansys®. During this process the design variables can be optimized such that the performance of the MEMS structure is improved.

The following subsections describe the primary components of the proposed software tool. Section 3.2.1 illustrates the Matlab® and Ansys® interface. This is
followed by a brief description of the Graphical User Interface (GUI) in Section 3.2.2. Along with these features a novel result validation parameter is introduced in this research which is called confidence factor. This factor is described in Section 3.2.3.

3.2.1 Matlab® - Ansys® interface

In the proposed software tool an interface module between Matlab® and Ansys® is developed. The motivation for developing such an interface is the fact that the both these tools are very powerful in their respective areas. Matlab® is known for its flexibility and easy-to-use architecture that allows the user to access complex optimization algorithms that are either built-in or user-defined. On the other hand, Ansys® is known for its ability to handle finite element analysis. As a result, the proposed tool was developed in Matlab® in which Ansys is called to simulate finite element analysis whenever necessary.

When the user inputs the dimensions of the MEMS structure under consideration along with the fabrication dependent data and the type of loading conditions (either structural or thermal loads), an Ansys® batch file is created through the proposed interface. The generated batch file can perform non-linear two-dimensional steady state or transient analysis. One must note that, though, in the current setup all the simulations are restricted to use Plane 82 solid element and Newton-Raphson method. The software tool can be very easily modified to accommodate other elements and solution techniques.

3.2.2 Graphical User Interface (GUI)

In the proposed software tool a GUI is developed in Matlab® in order to enter the process-dependent data and test structure information. The distinctive features of the GUI
include adaptability, flexibility, and transparency. There is no rigidity as regards the type of structure that can be studied, the plant, tool, material that can be used in the fabrication, or the kind of learning or searching techniques that can be employed for training. The GUI is able to encompass all parameters associated with the determination of the desired material property to create a model of the MEMS structure and to provide an accurate estimation of the desired property. Transparency is assured at every step to minimize human error.

This interface consists of three modules: Data Entry, Training, and Testing. Figure 3.4 illustrates the flow of information between the three modules.

The Data Entry module collects information from the user regarding the fabrication and geometry of the MEMS structure under study. The Training module is used to train the data obtained from the previous module. The Testing module tests samples generated at the data entry step based on the learning and searching techniques used during the training. These modules are described in detail below.
3.2.2.1 Data entry module

The Data entry module serves as a database of information. Figure 3.5 illustrates a screen shot of this module. This is the section which defines the material property to be extracted. In this section information is gathered from the user about the fabrication process and dimensions of the test structure.

**Figure 3.5: Screenshot of the data entry module in STEAM**

A single run of this module creates one sample of a test structure. A dataset is a collection of samples of the same kind of MEMS structures fabricated at a single plant, using the same materials and tools but varying in geometry. The flexibility of the GUI lies in the fact that it enables the user to either extract information from a list of existing plants and test structures, or enter new data. The Data Entry module includes a section
which elicits details of the structure under study. Each test structure is assumed to be composed of blocks. A block is a bounded area comprising of a single material. All information regarding the test structure is stored block-wise. The aforementioned section tags each block with a unique number which act as an identifier. One of the key features of this section is the ability to fix multiple feedback or control parameters which are obtained from various metrology tools during the actual fabrication of the test structure. These parameters are provided by the user and are used in the learning stage to minimize errors so that the obtained output conforms to the desired output.

Since the test structure is divided into blocks, the next section of the module elicits geometric information of each block. This section is subdivided into two hierarchical levels. The lower level is that of the edge, while the higher level is that of the block. At the lower level, the user is prompted to enter the co-ordinates of the endpoints of each edge that makes up the block and simultaneously provide information as regards the loading conditions of the corresponding edge. Loading conditions may include displacement (i.e. degrees of freedom), pressure, etc. This is one of the highlights of the module as it facilitates the creation of any kind of test structure and also allows for modeling of the loads to which each edge is subjected. The GUI also provides the user with the ability to input loading conditions which do not previously exist in the database thus enabling the creation of a near perfect model of the actual structure.

Each block is defined on the basis of its geometry which is entered at the edge level, the material it is composed of, the tool used for fabricating it and the recipe used for fabrication. As a result of the fabrication process, new parameters (e.g. stress) may come into effect. The GUI provides an option of including these fabrication-induced
parameters which are used during the training process for accurate modeling of the structure. The user is free to select these parameters from an existing list or define new parameters. The GUI creates a visual representation of the test structure defined by the user so as to increase transparency. Such a transparency exists at the edge as well as the block levels. The input into this module is stored and can be used later for the purpose of training or testing.

3.2.2.2 Training module

In this module (Figure 3.6) the user is prompted to define the test structure to be used for the training process.

![Figure 3.6: A screenshot of the training module](image-url)

Figure 3.6: A screenshot of the training module
This is done by selecting a dataset. Each dataset represents a collection of test structures identical in all respects except geometry and loading conditions. On picking a particular dataset, the samples that make up the dataset are made available for selection. At the same time information as regards the materials that comprise the test structure and the tools used for fabrication of the various blocks are also displayed. This again demonstrates the transparency of the GUI. The user can select any number of samples for the purpose of training. The Training module provides the user with an option for changing the bulk values of the material properties of the materials associated with the selected test structure. The user can input new material properties to improve modeling accuracy. If the user does not assign new bulk values or enter new material properties, the existing set of material properties and their corresponding values are chosen by default.

Based on the learning and searching technique chosen by the user, the training of the selected samples is done. The search technique generates the effective values of the material properties of the materials comprising the test structure. Effective material properties are computed using search techniques such as 2D search and genetic algorithms. Detailed descriptions on the various search techniques that can be used are presented in Chapter 4. The software tool also provides an option to define the various parameters in the search and learning techniques. Figure 3.7 illustrates the parameter modification module for search and learning technique. Using this feature, parameters such as learning rate, number of epochs, and tolerance can be modified for each soft computing technique.
The learning techniques are utilized to study the relationship between the geometric and fabrication parameters for the entire dataset. The learning techniques built into the proposed system were Radial Basis Functions Networks (RBFN) and neural networks [38-40]. However, due to the availability of other search techniques as well as non-parametric based learning techniques, this module enables the user to add to the existing list of searching and learning techniques.

![Parameter modification module for search and learning techniques](image)

**Figure 3.7: Parameter modification module for search and learning techniques**

The information input into the Training module is sent to the MATLAB® - ANSYS® interface from where it passes on to ANSYS® for processing. The developed empirical models can then be utilized in the testing module, which is described below.
3.2.2.3 Testing module

Figure 3.8 illustrates a screenshot of the Testing module. This module is used for testing samples that have been generated by the Data Entry module. Not all samples of a given dataset may be used for training.

![Testing Module GUI](image)

**Figure 3.8: A screenshot of the testing module**

The GUI provides the flexibility of selecting untrained samples for testing. This is used to validate the efficiency of the learning technique used. In this module, the user can select a particular dataset from a list of existing datasets. Based on this selection the corresponding samples populate another list. From this list any number may be chosen for the purpose of testing. This requires the user to specify the searching and learning technique used for training. The input information is passed on to the MATLAB® -
ANSYS® interface from where control is given over to ANSYS® which performs the required processing.

Apart from the above described features, this research introduces a novel confidence factor that quantifies the accuracy of the results output in the testing module. This factor is described in the following section.

### 3.2.3 Confidence factor

State of the art CAD tools for MEMS, while estimating the material properties of thin films, consider only the fabrication process parameters and bulk values [21-28]. In the process, they assume that material properties are only function of deposition technique and ignore the dependence on the tool as well as fabrication facility. In the literature, it has been shown that such an assumption is not valid [5, 15]. This is because apart from the process variables, factors such as orientation of the deposition surface relative to the direction of coating and substrate temperature which are very specific to the fabrication tool in a facility affect the material properties of thin films [10]. As a result, any generalization could result in an inaccurate prediction of the mechanical behavior.

In order to overcome this limitation, in this research, a novel parameter called confidence factor that validates the estimates predicted by the empirical models was developed. The rationale behind emphasizing this parameter is that many times fabrication data may not be available during the design process. This limitation results in inaccurate prediction. Despite this disadvantage, it may be acceptable in few situations to perform steady state analysis. Under such circumstances the MEMS designer would be interested to know the percentage error in the design. Other applications of the
confidence factor is in estimating the amount of training data required for learning the behavior to a desired accuracy.

Due to the uncertainty and complexity in the design and development of the confidence factor, this research proposes the use of fuzzy logic. This is because fuzzy logic provides an effective framework for dealing with the problem of knowledge representation in an environment of uncertainty and imprecision [41-42]. It was specifically designed to mathematically represent uncertainty and vagueness and provide formalized tools for dealing with the imprecision intrinsic to many problems.

Fuzzy logic systems address the problem of imprecision of the input and output variables by defining them with fuzzy sets that can be expressed in linguistic terms (e.g., low, medium and high) [41, 42]. These systems are developed such that they allow far greater flexibility in formulating system descriptions at the appropriate level of detail. This means that complex process (usually nonlinear) behavior can be described without the precise mathematical formulation of the problem. For a detailed description of fuzzy logic, readers are directed to the following references [41, 42]. The following section illustrates the various parameters of the fuzzy confidence factor.

Figure 3.9 illustrates the block diagram of the fuzzy confidence factor. As illustrated in this figure, the input variables to the fuzzy system are the fabrication facility, complement of mean square error (CMSE), and the number of datasets used for training. The output of the fuzzy system is the confidence factor in percentage value.

The following section illustrates the various fuzzy parameters that define the confidence factor. Section 3.2.3.1 describes fuzzy membership functions for the various
input and output variables and Section 3.2.3.2 describes the fuzzy rule base system and the inference engine.

Figure 3.9: Block diagram of the fuzzy confidence factor

3.2.3.1 Fuzzy membership functions

Input and output variables of the confidence factor are represented in fuzzy logic using membership functions and linguistic variables. As opposed to the classical set theory that can take one of only two values (zero and one) membership functions in a fuzzy set are a continuous function with a range of \([0, 1]\). On the other hand, linguistic variables are those fuzzy subsets that describe the input/output variable in terms of words from the natural language. In this research, triangular membership functions were used to represent the linguistic variables for the input/output variables. The following discussion illustrates the membership functions associated for the input/output variables.

The membership functions that describe the input variable “fabrication facility” are a combination of various fabrication parameters that can be used to deposit a thin
film. Table 3.1 illustrates the linguistic variables that describe this input variable. The fuzzy sets for these linguistic variables are obtained using expert knowledge.

Table 3.1: Linguistic variables of the input parameter “fabrication facility”

<table>
<thead>
<tr>
<th>Description</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material deposited in the same plant using the same tool and same recipe</td>
<td>SPSTSR</td>
</tr>
<tr>
<td>Material deposited in the same plant in the same tool but a different recipe</td>
<td>SPSTDR</td>
</tr>
<tr>
<td>Material deposited in the same plant using a different tool with same principle of deposition (example, CHA Evaporator vs CVC Evaporator)</td>
<td>SPDTSD</td>
</tr>
<tr>
<td>Material deposited in the same plant using a different tool with different principle of deposition (example, Oxide growth vs Oxide Deposition)</td>
<td>SPDTDD</td>
</tr>
<tr>
<td>Material deposited in a different plant using the Same tool (same make and model), same recipe</td>
<td>DPSTSR</td>
</tr>
<tr>
<td>Material deposited in a different plant using the same tool (same make and model) but a different recipe</td>
<td>DPSTDR</td>
</tr>
<tr>
<td>Material deposited in a different plant using a Different tool, with the same principle of deposition</td>
<td>DPDTSD</td>
</tr>
<tr>
<td>Material deposited in a different plant using a Different tool with the different principle of deposition</td>
<td>DPDTDD</td>
</tr>
</tbody>
</table>

The membership functions for the above described variables are illustrated in Figure 3.10.

![Figure 3.10: Fuzzy membership functions for the input variable “fabrication facility”](image)
The second input variable for the fuzzy system is the Complement of the mean square error (CMSE). This fuzzy variable is a measure of performance of the soft computing techniques that were used for generating the empirical models. As a result, one can say that the lower the CMSE value, more reliable is the empirical model. The fuzzy sets that are used to describe this input variable are ‘Low’, ‘Medium’, ‘High’ and ‘Very high’. Figure 3.11 illustrates the fuzzy membership functions for the input variable CMSE.

![Fuzzy membership functions for the input variable CMSE](image)

**Figure 3.11: Fuzzy membership functions for the input variable CMSE**

The third input to the fuzzy system is related to the number of data samples that were used for generating the empirical models. As discussed in Section 3.1.3, the number of datasets used in the training process plays a vital role in the generalization achieved by the soft computing techniques. Although it is difficult to know the amount of training data needed for each soft computing technique, it is a widely accepted fact that more training data enables better empirical models. In the proposed fuzzy systems the fuzzy membership functions that represent this variable are “Low”, “Medium” and “Large”. 
Figure 3.12 illustrates the fuzzy membership functions for this variable.

![Figure 3.12: Fuzzy membership functions for the input variable “datasets”](image)

Finally, the membership functions that represent the output variable confidence factor are, “Medium”, “Large” and “Very Large”. Figure 3.13 illustrates these membership functions.

![Figure 3.13: Fuzzy membership functions for the output variable “value”](image)
In this fuzzy system the membership function “Very Large” represents a confidence value in the range of 75% to 80%. Such high levels of confidence value are obtained in situations where the test conditions are very similar to the training data.

Given these membership functions, the next step involved in the development of the fuzzy system is to compute the fuzzy rule base system and the inference engine that would define the various fuzzy operators. These are illustrated in the following section.

### 3.2.3.2 Fuzzy rule base system and the inference engine

A fuzzy system is characterized by the inference method. The proposed fuzzy system was developed using the Mamdani minimum inference method in which the ‘and’ operator was represented by minimum operation and de-fuzzification was carried out using centroid defuzzifier [41]. This inference engine includes the rule base for the system, the above-described membership functions that are used for the fuzzification of the input and output variables and the method of de-fuzzification of output variables. The results for the rule base as well as the fuzzy surface are illustrated in Chapter 5.

The following chapter describes the working of the proposed methodology by estimating the effective Young’s Modulus of thin films using micro-machined bilayer cantilevers as test structures. Among the various mechanical properties, recent emphasis has been on understanding the Young’s Modulus of thin film materials [43]. This is due to the fact that several design issues such as resonant frequency, stiffness, and the accuracy of the finite element analysis are greatly affected by Young’s Modulus [43].
Chapter 4: Case study with Micro-machined Bilayer Cantilevers

Micro-cantilevers have been widely used in various applications such as micro-elastic joints, micro-grippers, micro-scanners, optical switches, and micro-relays due to their large out-of-plane deflections [9]. These large deflections are obtained as a result of the residual stresses induced by the fabrication techniques, especially in the deposition and growth processes [9, 31, 34]. These residual stresses are caused either due to the crystallographic flaw that are built into the coating during deposition process or due to the mismatch of the thermal expansion coefficient between the coating and the substrate [10, 11]. As a result, residual stresses influence the mechanical properties of thin films. Thus, determining these stresses plays an important role in characterizing the initial angle induced in the bilayer cantilevers (see Figure 5.1) which, in turn, can be used for extracting the effective Young’s Modulus of the thin film materials.

This chapter is organized as follows. The physical interpretation of the stresses that are developed during the thin film deposition process is highlighted in Section 4.1. This discussion is followed by the description of the fabrication of the test structures in Section 4.2. The mathematical representation of the mechanical behavior of the bilayer cantilevers is illustrated in Section 4.3. This chapter also illustrates the two possible approaches that can compute the effective material properties. The first approach, illustrated in Section 4.4 is based on extracting the material properties using finite element analysis and soft computing techniques. Finally, in Section 4.5 the second
approach is illustrated, emphasizes the development of analytical solutions with certain assumptions.

4.1 Physical interpretation

In thin film materials, large internal stresses are produced during the fabrication process [9-11]. As a result, understanding the mechanical behavior of thin films on substrates requires an understanding of the stresses in thin films as well as the mechanism by which the thin films deform [9].

Many researchers attempted to solve this problem by fabricating a bilayer cantilever that consists of a base layer and an actuating layer [9, 31, 34]. The fabrication process of bilayer cantilevers could consist of depositing thin films by evaporation. In the evaporation process, the material is deposited in layers. As a result there is a finite amount of stress that is produced by the top layer on the bottom layers. This stress translates to a stress gradient across the entire material which results in volumetric rearrangement [44-46]. In the literature, the reasons for the formation of this stress gradient have been attributed to the annihilations of excess vacancies, dislocations, and grain boundaries. These lead to densification, phase transformations, and composition changes that produce dilatational strains [44-46].

There is a growing amount of interest in understanding the physics behind the growth and travel of misfit dislocations in thin films. These are said to be responsible for plastic deformations of thin films on non-deformable substrates [44]. In the case of bilayer cantilevers, the large out-of-plane deflections of the beams are attributed to the strains produced by the lattice mismatch and dislocation travel towards the free end of the cantilever [44]. Using this theory, various models were developed that quantify the
internal stresses produced in thin films [44]. However, these models cannot be
generalized to all thin films because the fundamental assumption in these models is that
the thin films are epitaxial crystalline structures [44]. Recent studies indicate that this
assumption may not be valid in most cases due to the fabrication limitations [35, 36]. It
was found that process variables such as substrate temperature, working gas species and
their pressure, and orientation of the deposition surface relative to the direction of coating
affect the residual stresses in deposition [10]. As a result, there is a need for new
techniques that can estimate the material properties of thin films. The proposed
methodology aims at solving the above described problem using empirical analysis. The
following section illustrates the mathematical formulation for computing the various
factors that affect the Young’s Modulus of self-deformed bilayer cantilevers.

4.2 Fabrication of the test structures

As a proof of concept, Young’s Modulus of three thin film materials that are
Silicon-dioxide (SiO₂), aluminum and polyimide were studied. This was achieved by
fabricating four sets of micro-cantilevers at Semiconductor Microsystems Fabrication
Laboratory (SMFL) at RIT. The first three sets consisted of SiO₂- aluminum bilayer
cantilevers. In these three sets aluminum was deposited on top of SiO₂ thin films using
different types of deposition techniques. The first set consisted of aluminum that was
deposited using the evaporation technique. In this technique, an aluminum flash source
was used in a CHA Evaporator that was maintained at 6.5x 10⁻⁶ Torr. The second set was
fabricated by depositing aluminum using the sputtering technique. This deposition was
carried out in the presence of Argon at 15 psi, vacuum pressure at 1.3x10⁻⁵ Torr and RF
power at 2000 W. The third set of aluminum- SiO₂ cantilevers was fabricated using
similar process conditions as in the second set along with an additional process step called substrate heating. In this process the wafers were heated at 300 °C for 20 minutes before the pre-sputter and the actual deposition. Finally, the fourth set consisted of SiO₂-polyimide bilayer cantilevers. In all these cantilevers SiO₂ thin films were the base layers. This layer was deposited at a RF power of 265 Watts by flowing TEOS at 400 SCCM and Oxygen at 285 SCCM (@ 9 mTorr).

The fabrication process for the SiO₂ and aluminum cantilevers as well as SiO₂ and polyimide cantilevers involves four steps along with one lithography step. Figure 4.1 illustrates the fabrication process for these bilayer cantilevers.

![Figure 4.1: Process steps for fabricating bilayer micro-cantilevers: (a) SiO₂ and Aluminum, (b) SiO₂ and Polyimide](image)

The first step in the fabrication of these cantilevers was to deposit SiO₂ of desired thickness on top of a bare silicon wafer. This was followed by depositing the top layer which was aluminum or polyimide. In the case of SiO₂-aluminum cantilevers, aluminum thin films were deposited using two different techniques, namely evaporation and sputtering. In the case of SiO₂-polyimide cantilevers, polyimide thin films were deposited by spin coating and curing the polyimide precursor at 400 °C for 15 hours. The
The next step involved patterning and etching the aluminum layer or the polyimide to define the dimensions of the micro-cantilevers. Finally, micro cantilevers are released by etching the silicon below the SiO$_2$ in SF$_6$ plasma (flowing at 30 SCCM) for 60 to 90 minutes. The duration of etch is dependent on the thickness of the microcantilever beams. The physical dimensions of the beams as well as the tip deflections were then computed using the SEM and the optical microscope.

The following section describes the mathematical representation of the bilayer cantilevers that can correlate the experimental deflections to the effective material properties to produce useful empirical models.

### 4.3 Mathematical representation

Depending upon the dimensions of the beams and the amount of residual stresses induced into the actuating material, large out-of-plane deflections can be observed on the released cantilever beams. In order to understand this mechanical behavior of the cantilevers, let us first consider a thin film that was deposited on a thick substrate as illustrated in Figure 4.2.

![Figure 4.2: A two-layer system consisting of a thin film on a substrate](image-url)
Assuming that the two films are in the stress-free state just before deposition and the internal stresses that are developed in the composite structure are formed after deposition, the stress-strain behavior can be expressed by the following Equation 4.1 [46].

\[ \varepsilon = \frac{\sigma}{E} + \varepsilon_p + \varepsilon_T \]  \hspace{1cm} (4.1)

where \( \sigma \) is the uniaxial stress induced in the thin film, \( \varepsilon_p \) is the inelastic strain due to plastic flow and \( \varepsilon_T \) is the transformation strains caused due to the internal stresses.

In addition, since the two layers adhere perfectly, the displacements in the two films caused by the internal stresses in the thin film must be equal. This condition simplifies Equation 4.1 to give the stresses in the thin films [46].

\[ \sigma_f = E_f \left( -\varepsilon_p^f + \Delta \varepsilon_T \right) \]  \hspace{1cm} (4.2)

where \( E_f \) is the Young’s Modulus of the thin film. In this research we assume that the materials under consideration are linearly elastic. As a result in equation 4.2, the inelastic strain (\( \varepsilon_p^f \)) due to the plastic flow can be neglected [46]. This further simplifies the computation of the stresses in the thin films as given in equation 4.3.

\[ \sigma_f = E_f . \Delta \varepsilon_T \]  \hspace{1cm} (4.3)

For the composite structure illustrated in Figure 4.2, the substrate thickness is much greater than the film thickness. As a result of this fact, stresses in the substrate can be neglected and the stresses in the thin films can be given by the following equation 4.4 which is often known as Stoney’s formulae [46].
\[
\sigma_f = \frac{E_s \cdot h_s^2}{6 \cdot h_f \left(1 + \frac{h_f}{h_s}\right) \cdot \rho}
\]  

(4.4)

Hence given the radius of curvature \(\rho\) (which can be obtained experimentally), the Young’s Modulus \(E_s\) of the substrate (bulk value), the thicknesses of the substrate \(h_s\) and the film \(h_f\), the stresses \(\sigma_f\) in the thin film can be computed.

In order to compute the mechanical behavior of the thin films, equation 4.3 has to be solved. However, equation 4.4 consists of three variables and the solution can be obtained if two of the three variables are known. Given the stresses in the thin films, equation 4.3 can be solved by assuming either the Young’s Modulus or the relative transformation strains to be known. By doing so, the uncertainty in the fabrication process is modeled into the parameter that is unknown. A literature survey revealed that both techniques have been popularly used in the past and there was no standard methodology [31, 34, 35, 46].

Based on the above discussion, this research proposes two approaches that can be used for analyzing the mechanical behavior of thin films. They are the soft computing approach and the analytical approach. In the soft computing approach, the relative transformation strains are assumed to be known and empirical models are generated for Young’s Modulus of the thin films based on soft computing analysis and finite element modeling. In the analytical approach, Young’s Modulus of the thin films is assumed to be the bulk value and the uncertainty in the fabrication is modeled into the relative transformation strains. This technique utilizes mathematical concepts from elastic theory to derive expressions for relative transformation strains as well as generalized equations.
that compute the stresses in the thin films that have varying dimensions. The following sections illustrate the working of the two proposed approaches.

### 4.4 Soft computing approach

This approach emphasizes the use of soft computing techniques for estimating the material properties of the thin films using empirical analysis and finite element modeling. Figure 4.3 shows a simplified block diagram of the proposed technique (illustrated in Chapter 3) that is specific to the soft computing approach.

![Figure 4.3: Schematic of the proposed methodology as applied to soft computing approach](image)

As shown in Figure 4.3, after selecting the test structure, the various steps involved in this methodology are the identification of the various parameters that influence the material property under consideration, finite element modeling and
empirical model generation. The following sub-sections illustrate these steps in detail for the computation of Young’s Modulus of thin films using bilayer cantilevers.

4.4.1 Mathematical relationship

This investigation contains a general theory of bending of a bilayer cantilever subjected to uniform residual stresses. Figure 4.4 illustrates a schematic of a typical bilayer cantilever.

![Schematic of a bilayer cantilever]

Figure 4.4: Schematic of a bilayer cantilevers

Let all the internal stresses over the cross-section of material “1” be expressed as tensile forces $P_1$ with a bending moment of $M_1$. For material “2” let the internal stresses be represented as compressive forces, $P_2$, with a bending moment of $M_2$ respectively. Since the internal forces over any cross-section of the beam must be in equilibrium, the following can be assumed.

$$P_1 = P_2 = P$$  \hspace{1cm} (4.5)
\[ \frac{P \cdot h}{2} = M_1 + M_2 \] (4.6)

Applying the concepts of flexure rigidity from Beam Theory [22, 27] we can express the above equation as follows.

\[ \frac{P \cdot h}{2} = \frac{E_1 \cdot I_1 + E_2 \cdot I_2}{\rho} \] (4.7)

where \( \rho \) is the radius of curvature of the composite beam, \( E \) is the elastic modulus of the beam, \( I \) is the moment of inertia and \( h \) is the thickness of the composite beam. Let \( a_1 \) be the thickness of material “1” and \( a_2 \) be the thickness of material “2”, then \( h \) is given by \( a_1 + a_2 \). Assuming that the stress is uniform, we can express stress \( (\sigma) \) in terms of force \( (P) \) and cross sectional area \( (A) \).

\[ \sigma = \frac{P}{A} \] (4.8)

Moment of inertia, \( I \), for each layer is expressed given by the following equation 4.9.

\[ I_1 = \frac{w \cdot a_1^3}{12}, I_2 = \frac{w \cdot a_2^3}{12} \] (4.9)

Also using Beam Theory [32], one can compute the maximum static deflection \( (\delta) \) for a beam clamped at one end, which is expressed as follows.

\[ \delta = \frac{l^2}{2\rho} \] (4.10)

Substituting equations 4.8 and 4.10 in equation 4.7 and simplifying the equation, the following resultant equation 4.11 is obtained

\[ \frac{\sigma \cdot h \cdot (h \cdot w)}{2} = \frac{E_1 \cdot I_1 + E_2 \cdot I_2}{\frac{l^2}{2\delta}} \] (4.11)
Which can be further simplified to result in (4.12).

\[ \frac{\sigma \cdot h^2 \cdot l^2 \cdot w}{4 \cdot \delta} = E_1 \cdot I_1 + E_2 \cdot I_2 \]  \hspace{1cm} (4.12)

Now substituting equation 4.9 in 4.12 and using \( h = a_1 + a_2 \), the above equation can be further simplified to

\[ \frac{3 \cdot \sigma \cdot (a_1 + a_2)^2 \cdot l^2 \cdot w}{\delta} = E_1 \cdot a_1^3 + E_2 \cdot a_2^3 \]  \hspace{1cm} (4.13)

Assuming that the terms in equation 4.13 can be decoupled, we can extract the relationship of the elastic modulus with the other quantities. Thus the proportionality equation can be expressed as follows.

\[ E \propto (\sigma, l, a, \delta) \]  \hspace{1cm} (4.14)

The above described mathematical analysis illustrates that the Young’s Modulus of the thin film is independent of the width of the cantilever beams. However, this argument has been contested by Hou et al [9]. Experimental analysis of bilayer cantilevers of various dimensions illustrate that the width of the cantilever clearly affects the Young’s Modulus of thin films [9]. This is because the stresses induced in the cantilever (see Figure 4.4) are not limited to the X axis but are also present in the Z axis. Thus, this questions the existing models that estimate the Young’s Modulus of wide and slender beams of the same length [9]. As a result, in the proposed methodology, the width of the cantilevers is taken into account in estimating the Young’s Modulus. Also, as discussed in Section 4.1, residual stresses induced into the materials are to a large extent dependent upon the process variables. Thus, the relationship in the equation 4.14 is nonlinear and can only be estimated empirically. Hence the effective elastic modulus can be expressed as a function
of the beam dimensions, geometry, as well as the stress induced into the bilayer cantilevers during the fabrication process as illustrated in equation 4.15.

\[
E = f(\sigma, w, l, a, \delta)
\]  

(4.15)

Thus equation 4.15 becomes the relationship between the material property under consideration and the physical parameters.

The above described relationship was computed using an alternative technique called Principal Component Analysis. The following section describes this technique.

### 4.4.2 Statistical analysis

In order to compute the relationship between the various factors that affect the Young’s Modulus of thin films, a statistical technique called Principal Component Analysis (PCA) was implemented. PCA is a common parametric technique that is used for finding patterns in data of high dimension [48-49]. PCA involves a mathematical procedure that transforms a number of possibly correlated variables into a smaller number of uncorrelated variables called principal components. The first principal component accounts for as much of the variability in the data as possible, and each succeeding component accounts for as much of the remaining variability as possible [49]. As a result, in this technique multidimensional data sets are reduced to lower dimensions (without loss of information), and new meaningful variables can be identified. Please refer to references [48] and [49] for more information about PCA as well as its mathematical derivations.

The following discussion illustrates the procedure of implementing PCA for computing the relationship between the various factors that affect the Young’s modulus of thin films in this work.
Step 1: Collect experimental data

In this step all the possible parameters that affect the Young’s Modulus are identified and experimental data is collected. In our analysis experimental data obtained by fabricating evaporated aluminum on SiO$_2$ micro-cantilevers were used as test data (refer to Section 5.1.1 for fabrication details). Experimental data pertaining to length, width, and aluminum thickness of the beams, was recorded as column vectors in a test matrix along with the effective Young’s Modulus of aluminum thin film (computed using the 2D gradient search technique) and stress induced in the aluminum thin film. Table 4.1 illustrates the data set that was used in this analysis. In this table the length, width, thickness, and the effective Young’s Modulus of aluminum computed using the gradient search technique are represented by $L_B$, $W_B$, $T_B$, and $E_{al}^l$, respectively.

<table>
<thead>
<tr>
<th>$L_B$</th>
<th>$W_B$</th>
<th>$T_B$</th>
<th>$E_{al}^l$</th>
<th>Stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>(µm)</td>
<td>(µm)</td>
<td>(µm)</td>
<td>(MPa)</td>
<td>(MPa)</td>
</tr>
<tr>
<td>94.24</td>
<td>26.98</td>
<td>0.41</td>
<td>2188</td>
<td>27.4</td>
</tr>
<tr>
<td>489.8</td>
<td>61.44</td>
<td>0.39</td>
<td>2188</td>
<td>13.67</td>
</tr>
<tr>
<td>402.8</td>
<td>65.64</td>
<td>0.39</td>
<td>2188</td>
<td>13.67</td>
</tr>
<tr>
<td>205.8</td>
<td>62.64</td>
<td>0.39</td>
<td>2188</td>
<td>13.67</td>
</tr>
<tr>
<td>487.4</td>
<td>99.8</td>
<td>0.41</td>
<td>2188</td>
<td>35.92</td>
</tr>
<tr>
<td>100.8</td>
<td>47.62</td>
<td>0.41</td>
<td>4375</td>
<td>27.4</td>
</tr>
<tr>
<td>205.8</td>
<td>64.6</td>
<td>0.45</td>
<td>4375</td>
<td>55.49</td>
</tr>
<tr>
<td>301.4</td>
<td>41.8</td>
<td>0.41</td>
<td>4375</td>
<td>35.92</td>
</tr>
<tr>
<td>207.4</td>
<td>99.8</td>
<td>0.41</td>
<td>4375</td>
<td>35.92</td>
</tr>
<tr>
<td>485.8</td>
<td>62.3</td>
<td>0.45</td>
<td>6563</td>
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</tr>
<tr>
<td>156.6</td>
<td>51.2</td>
<td>0.45</td>
<td>19688</td>
<td>55.49</td>
</tr>
</tbody>
</table>

Step 2: Subtract mean

In this step the mean across each dimension is computed and this mean is subtracted from each of the data dimensions resulting in an adjusted test matrix.
Step 3: Calculate the covariance matrix and its corresponding eigenvalues and eigenvectors

Using Matlab predefined functions, covariance of the adjusted test matrix is computed. The resulted matrix is a fifth order square matrix. In order to extract the various characteristics in the data, eigenvalues ($D$) and eigenvectors ($V$) of the covariance matrix are computed and analyzed. The calculated values for $D$ and $V$ are as follows.

$$D = \begin{bmatrix}
0.1440 & 0 & 0 & 0 & 0 \\
0 & 0.1035 & 0 & 0 & 0 \\
0 & 0 & 0.0350 & 0 & 0 \\
0 & 0 & 0 & 0.1035 & 0 \\
0 & 0 & 0 & 0 & 0.1440 \\
\end{bmatrix}$$

$$V = \begin{bmatrix}
-0.5554 & 0.6894 & 0.4647 & 0.0147 & -0.0027 \\
-0.2145 & 0.3827 & -0.8118 & -0.3842 & 0.0296 \\
0.1079 & 0.0871 & 0.0023 & 0.0978 & 0.9855 \\
0.5502 & 0.2454 & 0.3166 & -0.7326 & -0.0100 \\
0.5754 & 0.5571 & -0.1572 & 0.5532 & -0.1667 \\
\end{bmatrix}$$

A close look at the eigenvalues reveals that among the five variables a clear relationship can be obtained only for four variables since the last eigenvalue is very small compare to others. In order to determine these four variables the feature vectors need to be analyzed.

Step 4: Feature vector and analysis

A feature vector is a matrix which has eigenvectors as columns [48]. In PCA the eigenvector corresponding to the highest eigenvalue is the principal component of the data set and the significance of the remaining eigenvectors decreases as the eigenvalue
deceases [48]. As a result a feature vector comprising of all the eigenvectors contains information of the entire data set. However by eliminating the lesser significant eigenvectors, the data can be recreated within acceptable error percentages. The following Figures 4.5- 4.10, illustrate the error in each of the variables ($L_B, W_B, T_B, E_{ab}^l$, and Stress) for different sizes of the feature vector.

**Figure 4.5: Error in $L_B$ for different sizes of feature vector**

**Figure 4.6: Error in $W_B$ for different sizes of feature vector**
Figure 4.7: Error in $T_B$ for different sizes of feature vector

Figure 4.8: Error in $E_{ad}^I$ for different sizes of feature vector

Figure 4.9: Error in Stress for different sizes of feature vector
The above figures clearly demonstrate that the data set illustrated in Table 4.1 can be characterized by the eigenvectors corresponding to the highest three eigenvalues. Also since the rows in the feature vector correspond to the various parameters, analyzing the values in the rows shall indicate the relationship between the various parameters. Thus, in the principal component the parameters $L_B$, $E_{dl}$, and Stress have a significant contribution when compared to the $W_B$, $T_B$. This implies that the effective Young’s Modulus is primarily a function of the length of the cantilevers and the stress induced in the fabrication and is not affected by the thickness of the aluminum layer and the width of the cantilever. Since in these experiments (refer to Section 5.1) the thickness of the aluminum layer has been kept constant, the above conclusion can be justified. However, more samples have to be obtained and analyzed before any conclusions are made.

The above discussion clearly illustrates the working of PCA as applied to the problem at hand. Although PCA is a very useful technique, the following are its limitations [49].

PCA assumes:

1. The relationship between the various parameters is linear.
2. Mean and Variance are sufficient statistics to describe the problem at hand. This assumption is valid only if the mean and the variance corresponds to a probability distribution.
3. Large variances have important dynamics. This assumption leads to belief that the data has high SNR.
4. The principal components are orthogonal. This assumption gives way to simplification of the problem with linear algebra decomposition techniques.
These assumptions clearly illustrate that PCA is a good starting point for this research. However, more advanced non-parametric techniques are required to develop relationship between the various parameters. As a result, the proposed technique aims to discover this approximate function through experimental data and model generation algorithms using CAD tools such as Ansys® and Matlab® for FEA and soft computing techniques, respectively. The following section describes this process in detail.

4.4.3 Finite element modeling

Large out-of-plane rotations of the cantilever beams were modeled in Ansys®, a finite element analysis software tool. Simulations were performed in the two-dimensional structural analysis mode using the Plane 82 solid element. The solution was computed by using non-linear steady state static analysis which uses the Newton-Raphson method along with an initial stress value.

Effective Young’s Modulus values were computed for aluminum and SiO₂ for each data set obtained from the fabrication results. These values were computed by modifying the bulk values until the simulations matched the experimental values (See Figure 4.3). A literature survey as well as previous simulation results indicated that the search space was material dependent [35, 36]. It was found that Young’s Modulus for aluminum varied between 2 GPa to 70 GPa (bulk value) and TEOS varied between 10 GPa to 73 GPa [35]. These results are discussed in detail in Chapter 5. Due to this wide spread in the search space, intelligent search techniques (soft computing methods) are desired for faster results with better accuracy. In this analysis, two types of search techniques, two dimensional gradient search technique and micro-genetic algorithms,
were explored and their performance was compared. The following sub-section briefly describes these two algorithms.

### 4.4.3.1 Two dimensional gradient search technique

This search technique is commonly used in optimization problems where the solutions cannot be obtained using analytical methods [30]. Figure 4.10 is a pictorial representation of the working of 2D search technique in computing the effective values of Young’s Modulus.

![Figure 4.10: Implementation of the 2D search technique](image)

In this technique, the effective Young’s modulus of the material is computed using an iterative gradient descent vector. The following equations describe this behavior mathematically.

\[
E_{\text{eff}, \text{itr}}^1 = E_{\text{eff}, \text{itr}-1}^1 \pm \nabla E_{\text{const}}^1 \times E_{\text{eff}, \text{itr}-1}^1 \\
(4.16)
\]

\[
E_{\text{eff}, \text{itr}}^2 = E_{\text{eff}, \text{itr}-1}^2 \pm \nabla E_{\text{const}}^2 \times E_{\text{eff}, \text{itr}-1}^2 \\
(4.17)
\]
where $E^{1}_{eff,itr}$ and $E^{2}_{eff,itr}$ represent the current effective Young’s modulus for the top layer material (either aluminum or polyimide) and the base layer material (TEOS), respectively. The symbols $\nabla E^{1}_{const}$ and $\nabla E^{2}_{const}$ are the constant gradients that provide direction and step size of movement. In this analysis, $\nabla E^{1}_{const}$ was fixed at 0.7 for material “1” and $\nabla E^{2}_{const}$ was fixed at 0.12 for material “2”. The working of this technique is as follows.

The algorithm starts by assuming bulk property values of the materials for $E^{1}_{eff,1}$ and $E^{2}_{eff,1}$. These effective values are then used in the finite element analysis to compute the tip deflection of bilayer cantilevers, which is the feedback parameter for this analysis. If the error between the simulations and the experimental values is greater than 5%, a new set consisting of four combinations of $E^{1}$ and $E^{2}$ are computed using equations 4.16 and 4.17 which is shown by point “A” in Figure 4.10. Note that the four combinations are obtained such that the effective values of $E^{1}$ and $E^{2}$ increase or decrease simultaneously or $E^{1}$ changes keeping $E^{2}$ constant or $E^{1}$ is constant and $E^{2}$ changes. By doing so, the algorithm searches for a better solution in the neighborhood of the previous best solution. The four combinations of the effective values are then analyzed in finite element analysis and ranked based on the tip deflection. The combination that results in the least error is used for the next iteration. The above process is repeated until the error between the deflection computed by the effective values and the experimental values is less than 5%. The above description clearly indicates that this is a fairly straightforward and easy to use linear technique. The following section describes an alternative search technique that is non-linear and is based on genetic algorithms.
4.4.3.2 Micro-genetic algorithm (MGA)

Another popular non-linear search technique is the genetic algorithm [50-51]. This algorithm is classified under the umbrella of global search heuristics that are a particular class of evolutionary algorithms which use techniques inspired by biology such as selection, mutation and crossover [50]. In this technique the search space is generally binary coded and genes are formed by expressing the design variables in the binary form. A combination of these genes forms a chromosome that belongs to a population that represents the candidate solutions. The evolution starts from a large population of random chromosomes and happens in generations. In each generation, the fitness of the whole population is evaluated; multiple individuals are stochastically selected from the current population, and modified to form a new population which is then used in the next iteration of the algorithm. This process is iterated until the fitness evolutions meet the allowable tolerance [50]. Although this technique has been proved to yield good results, its major drawback is the massive amount of computational power and time required to reach a solution [50-51].

A modification of this technique is the micro-genetic algorithm (MGA) [50]. Just as in GA, the MGA works with binary coded population. However, in MGA only five parents are used in any generation and the successive generations are computed with the crossover of two parents. The reduced population size was achieved by improving the crossover technique. In MGA new populations are generated by transferring the chromosomes with the best solution to the next generation and generating the others randomly [50]. The following discussion illustrates the application of MGA in computing the effective material properties.
In accordance with the MGA, we use 5 parent chromosomes. Each parent chromosome is a pair of effective Young’s Modulus for materials 1 and 2. The effective Young’s Modulus values are encoded as an integer between 0 and 31. The value is used to reference a lookup table that contains 32 quantized effective Young’s Modulus values between 2 GPa and the bulk value of the material. When the actual crossover or mutation needs to be carried out the integer values that represent the effective Young’s Modules of the materials are extracted and converted to two 16 bit binary data that together constitute a parent chromosome. For the fitness computation, we convert the chromosomes back to the analog form (with the help of the lookup table) and compute the tip deflection of the bilayer cantilever using finite element analysis. The error between the simulation and the experiments are computed for each chromosome. Since the best fitness is achieved with the least error, we sort the parent chromosomes in ascending order. At this point crossover and mutation algorithms are applied. Figure 4.11 illustrates the crossover and new parent formation in MGA.

Figure 4.11: Implementation of the Micro-genetic algorithm
As shown in Figure 4.11, parents with the best and the second best fitness are transferred to the next generation. The remaining three child chromosomes are formed by a two point crossover of the five parents. Mutation has also been introduced into the code in order to allow the potential exist from local minima. The mutation in this case has been carried by inverting the MSB of Child 1 and LSB of child 2 randomly. The above iteration is repeated with the new generation until the error between the deflections obtained using the effective values and the experimental values is less than 5%.

The following section illustrates the two empirical estimation techniques that were implemented in this research.

### 4.4.4 Empirical estimation techniques

As described in Chapter 3, due to lack of proper understanding of the physical phenomena that relate the device dimensions and process dependent parameters, developing analytical techniques may be a complex task. In this case of bilayer cantilevers the various factors that influence the Young’s Modulus are the dimensions of the beam and the initial stress induced into the thin films during deposition. Due to the highly non-linear relationship between the parameters, effective models can be developed only by empirical models.

Among the various techniques reported in the literature for empirical models in multi-dimensional space, one dimensional radial basis function networks (1D-RBFN) as well as neural networks (NN) are the most popular methods [38-40]. These networks compute a surface in the multi-dimensional space that best fits the training data. A detailed description of these networks is given below.
4.4.4.1 Neural networks

Artificial neural networks were conceptualized to imitate the human brain in order to solve complex optimization issues in the engineering and sciences fields [38, 40, 52]. These networks are known for their ability to learn a particular solution to a problem and then apply it towards finding a general solution. A typical neural network consists of three layers: input layer, hidden layer and output layer. This configuration is often called multilayer perceptron network. Nodes in each layer are represented by a sigmoid function. Equations 4.18 and 4.19 illustrate the mathematical representation of the hidden nodes and the output nodes respectively.

\[ h(m) = \text{sigmoid}(\sum_{i=1}^{n} x_i w_{i,m}) \]  

where \( h(m) \) represents the \( m^{th} \) hidden node’s output, \( x_i \) is the \( i^{th} \) input, \( w_{i,m} \) are corresponding weights of the neural network and \( n \) is the number of input variables. The effective Young’s modulus is computed as follows.

\[ \hat{E}(m) = \text{sigmoid}(\sum_{i=1}^{p} \sum_{j=1}^{q} h_{i,j} w_{i,j,m}) \]  

Where \( p \) is the number of hidden nodes and \( q \) is the number of output nodes. The most popular technique that is used for training these networks is the back propagation algorithm [40, 52]. In this algorithm the weights of the network are iteratively optimized to learn the relationship between the input and output variables. These weights are optimized using a simple easy-to-use gradient descent technique [40]. Due to these advantages this algorithm was used to learn the relationship between the input parameters
and the effective material properties. This algorithm was implemented in Matlab® (Neural Network toolbox).

Figure 4.12 illustrates the schematic architecture of back-propagation algorithm that was applied to this research work. As shown in Figure 4.12, the inputs to the network are the physical dimensions of the beams as well as the fabrication-induced parameters such as induced stress. The output of the network is the effective Young’s modulus.

**Figure 4.12: Architecture of the back propagation based neural networks**

The architecture of neural network was case dependent and was determined empirically. As a result, the number of nodes in the hidden as well as the output layers was not constant for all the models. On an average, 6 hidden nodes and 5 output nodes were used in this analysis. The other neural network parameters that were used in the training process are the learning rate, goal and number of epochs. The networks were trained with a learning rate of 0.5, goal of 1e-5 and 3000 epochs. Another popular learning technique is the radial basis function networks. This is discussed in the following section.
4.4.4.2 One-dimensional radial basis functions networks

In the literature, for empirical models in multi-dimensional space, Radial Basis Functions (RBF) networks are the most popular [38, 39]. These networks compute a surface in the multi-dimensional space that best fits the training data. In this analysis, a modified version of RBF called one dimensional radial basis functions (1D-RBF) is used for modeling due to advantages such as sensitivity to the inputs and outputs [38, 39]. As illustrated in Figure 4.13 the 1D-RBF networks consist of three layers: input layer, hidden layer, and the output layer.

![Architecture of 1D- radial basis function networks](image)

Figure 4.13: Architecture of 1D- radial basis function networks

The input layer consists of four elements which are stress, length, width, and thickness of the beam. The outputs of the hidden RBFs used in this network are Gaussian in form and are given by equation 4.20.
where \( p \) is the number of input elements, \( M \) is the number of RBFs associated with each input, \( c_{pk} \) is the center of the \( k^{th} \) RBF for the \( p^{th} \) input vector, and \( \sigma_{pk} \) is the dilation (spread) of the \( k^{th} \) RBF for the \( p^{th} \) input vector. The output layer weights, \( w \), are calculated using the following equations.

\[
F^+ = \left( F^T \cdot F \right)^{-1} \cdot F^T \quad \text{and} \quad w = F^+ D_{out}
\]

where \( D_{out} \) is the desired output which is the ANSYS® estimate of the Young’s Modulus. The output of the network is the estimated Young’s Modulus (\( \tilde{E} \)) which is the multiplication of the weights (after training) and the outputs of the RBFs.

In this analysis, the number of RBFs associated with the input variable is different for each data set. This value was designed empirically. In the case of evaporated aluminum on TEOS cantilevers, it was found that 7 RBFs gave the optimal result. As a result, each input node was associated with 7 RBFs. Also, the center of the RBFs was chosen to be the training set with the dilations set to average distance between the center and the input vector.

The following section describes the second approach that is based on computing the relative transformation strains for each process condition. This technique is purely analytical in nature and assumes that the Young’s Modulus of the material will be the bulk value.

### 4.5 Analytical approach: Relative transformation strains

This approach proposes to analyze the mechanical behavior of bilayer cantilevers using the concepts of elastic theory [46]. The fundamental assumptions in this technique
are that Young’s Modulus of the thin films remains unchanged from the bulk value and the internal stresses developed during the deposition cause transformation strains that deform the composite structure. Hence by modeling the transformation strains for each process, the mechanical behavior of the bilayer cantilevers can be predicted.

In this analysis, mathematical models are extracted by analyzing the edge stresses at the interface of the bonded films. As described in Section 4.1, thin films are subjected to large internal stresses during the deposition phase. In order to understand the effect of the internal stresses on the films, let us consider two thin films that are in a stress-free state before bonding. Once bonded there is an internal biaxial stress in the layers that causes transformation strains at the interface which in turn causes the films to deform until an equilibrium state is reached. Hence by analyzing the edge stresses at the interface, one can compute the transformation strains in the layers. However, these stresses cannot be computed easily as there are several non-linear effects that are difficult to account for [46]. As a result, these stresses are replaced by an equivalent force $F$ and a corresponding bending moment $M$. Also, according to the St. Venant’s principle, the edge loading effects decay to negligible values from the edges [46]. As a result, in order to analyze these bilayer cantilevers, an equivalent free body is developed that computes the forces and the moments at the center of the beams. These free body diagrams are illustrated in Figure 4.14.

Let $\rho$ be the radius of curvature of the bonded two layer films and $E_1$ and $E_2$ be the bulk values of the Young’s Modules of layers 1 and 2. Also, Let $I_1$ and $I_2$ be the moments of inertia of the layers 1 and 2, respectively, which are given by equation 4.22.
\[ I_1 = \frac{w \cdot h_1^3}{12}, I_2 = \frac{w \cdot h_2^3}{12} \] (4.22)

Since the radius of curvature of both layers is the same, the equivalent forces and moments in the two layers can be expressed as follows.

\[ \frac{F \cdot h_1}{2} - M = \frac{E_1 \cdot I_1}{\rho} \] (4.23)

Equations 4.23 and 4.24 consist of two unknowns. As a result, these equations can be solved for \( F \) and \( M \) given in equations 4.25 and 4.26, respectively.

Figure 4.14: Free body diagrams of the bilayer cantilevers [53]

\[ \frac{F \cdot h_2}{2} - M = \frac{E_2 \cdot I_2}{\rho} \] (4.24)
\[
F = 2 \cdot \frac{(E_1 \cdot I_1 + E_2 \cdot I_2)}{\rho \cdot (h_1 + h_2)}
\]  
(4.25)

\[
M = \frac{(E_2 \cdot I_2 \cdot h_1 - E_1 \cdot I_1 \cdot h_2)}{\rho \cdot (h_1 + h_2)}
\]  
(4.26)

In order to compute the stresses at various locations of the thin films, let us consider that the only significant non-zero stresses in the films are in the x-axis. Hence the stress at the top and bottom of the two layers can be computed using the following equations (4.27 to 4.30).

\[
\sigma_{1}^{\text{top}} \equiv \sigma_1 \left( y_1 = \frac{h_1}{2} \right) = \frac{F}{h_1 \cdot w} + \frac{(M - 0.5 \cdot F \cdot h_1) \cdot h_1}{2 \cdot I_1}
\]  
(4.27)

\[
\sigma_{1}^{\text{bot}} \equiv \sigma_1 \left( y_1 = -\frac{h_1}{2} \right) = \frac{F}{h_1 \cdot w} - \frac{(M - 0.5 \cdot F \cdot h_1) \cdot h_1}{2 \cdot I_1}
\]  
(4.28)

\[
\sigma_{2}^{\text{top}} \equiv \sigma_2 \left( y_2 = \frac{h_2}{2} \right) = -\frac{F}{h_2 \cdot w} - \frac{(M + 0.5 \cdot F \cdot h_2) \cdot h_2}{2 \cdot I_2}
\]  
(4.29)

\[
\sigma_{2}^{\text{bot}} \equiv \sigma_2 \left( y_2 = -\frac{h_2}{2} \right) = -\frac{F}{h_2 \cdot w} + \frac{(M + 0.5 \cdot F \cdot h_2) \cdot h_2}{2 \cdot I_2}
\]  
(4.30)

Given the stresses at the interface of the two layers, the transformation strains can be computed as follows. Let the only significant non-zero component of the strains be in x-axis. Also, let \( \Delta \varepsilon^T = \varepsilon_2^T - \varepsilon_1^T \), where \( \Delta \varepsilon^T \) is defined as the relative transformation strain between the two layers. In order to compute this relative transformation strain, let us compute the strains at the interfaces of the two layers. These are expressed in equations 4.31 and 4.32.

\[
\varepsilon'_1 = \varepsilon_1 \left( y_1 = -\frac{h_1}{2} \right) = \frac{\sigma_{1}^{\text{bot}}}{E_1} + \varepsilon_1^T
\]  
(4.31)
\[
\varepsilon'_2 = \varepsilon_2 \left( y_2 = \frac{h_2}{2} \right) = \frac{\sigma_{2 \text{top}}}{E_2} + \varepsilon'_2
\]  
(4.32)

Since the displacements are continuous, \( \varepsilon'_1 = \varepsilon'_2 \), equations 4.31 and 4.32 can be equated and simplified by substituting 4.25, 4.26, 4.28, and 4.29 to result in the following equation.

\[
\Delta \varepsilon^T = \frac{2 \cdot (E_1 \cdot I_1 + E_2 \cdot I_2) \cdot \left( \frac{1}{E_1 \cdot h_1 \cdot w} + \frac{1}{E_2 \cdot h_2 \cdot w} \right) \cdot (h_1 + h_2)}{\rho \cdot (h_1 + h_2)} + \frac{2 \cdot \rho}{2 \cdot \rho}
\]  
(4.33)

Thus relative transformation strain can be computed using equation 4.33. In addition to this equation, researchers at RIT developed the relative transformation strains from Stoney’s Approximation which is illustrated in equation 4.34 [53].

\[
\Delta \varepsilon^T \approx \left( \frac{E_2}{E_1} \right) \cdot h_2^2 + \frac{h_2^2}{6 \cdot \rho \cdot h_1 \cdot \left( \frac{h_1}{h_2} + 1 \right)} + \frac{h_2}{6 \cdot \rho \cdot (h_1 + h_2)} + \frac{h_2}{2 \cdot \rho}
\]  
(4.34)

As seen in these equations (4.33 and 4.34), the relative transformation strains are functions of the dimensions of the beams as well as the fabrication process given by the radius of curvature. Thus the relative transformation strains are unique to a process and a recipe. As a result, empirical models can be developed that correlate the dimensions of the beam and the relative transformation strains to generate the effective material properties.

The following chapter illustrates the fabrication and simulation results that validate the proposed techniques and a novel micro-mirror.
Chapter 5: Results and Discussion

The lack of material properties in the micro-scale domain has motivated this research to develop a methodology that computes reliable effective material properties of thin film materials. As described in Chapter 4, two approaches were proposed that develop empirical models based on either soft computing techniques or analytical techniques. This chapter illustrates the results that validate the claims of the proposed methodology as well as the novel fuzzy confidence factor.

This chapter is organized as follows. Section 5.1 describes the fabrication results for the bilayer cantilevers. Section 5.2 provides a comparison of the finite element simulations of the mechanical behavior predicted by the bulk values to the experimental values. In this section the working of the empirical models that are developed using various soft computing techniques are also illustrated along with the performance analysis. In addition to the above-described performance analysis, the empirical models were validated by fabricating and simulating a novel MEMS mirror. Section 5.3 describes the second proposed approach that is based on analytical modeling of the mechanical behavior. This section deals with computation of radius of curvature, stresses in the thin films at various locations and modeling the relative transformation strains. Finally, in Section 5.4 the working of the fuzzy confidence factor is described with an example.

5.1 Fabrication results

Bilayer cantilevers comprised of aluminum and TEOS as well as polyimide and SiO₂ were fabricated using the process described in Chapter 4. In the case of aluminum-
SiO₂ cantilevers, two sets were generated based on the technique used for depositing aluminum thin films. The first set of aluminum- SiO₂ cantilevers were fabricated by evaporating aluminum (tool used was CHA Evaporator) on TEOS based SiO₂ which was deposited using plasma-enhanced chemical vapor deposition (tool used was Applied Materials P5000) [37]. In the second set, aluminum was sputtered (tool used was CVC601) on TEOS [37]. These two sets were fabricated to study the effects of change in process/recipe on the material properties of thin films as well as to validate the results of the confidence factor.

In all the above-listed sets of cantilevers, residual stresses were developed in the actuating layer (i.e., the top layer; either aluminum or polyimide) during the deposition process that resulted in the out of plane deflection of the cantilevers. As described in Chapter 4, the various parameters that affect the Young’s Modulus of thin films are the physical dimensions of the test structure as well as the stress induced in the actuating layer. As a result, using various metrology tools the stress is measured. The metrology of the beams was obtained using tools such as the scanning electron microscope (SEM), optical microscope, as well as a surface scan profilometer [37]. The stress induced in the actuating layer (aluminum or polyimide) was measured using the Tencor® profilometer before patterning and etching [37]. The following sub-sections illustrate the experimental data obtained from the four sets of bilayer cantilevers.

### 5.1.1 Aluminum- SiO₂ bilayer cantilevers

Table 5.1 illustrates the stress measurements, the static deflection, and the dimensions of the micro-cantilever beams comprised of evaporated aluminum on SiO₂. In
Table 5.1: Micro-cantilever beams consisting of SiO₂ and evaporated aluminum

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Stress Al (MPa)</th>
<th>L_B (µm)</th>
<th>W_B (µm)</th>
<th>d_B (µm)</th>
<th>T_B Al (µm)</th>
<th>T_B SiO₂ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>27.4</td>
<td>94.24</td>
<td>26.98</td>
<td>53.78</td>
<td>0.41</td>
<td>0.51</td>
</tr>
<tr>
<td>2</td>
<td>27.4</td>
<td>100.8</td>
<td>47.62</td>
<td>39.7</td>
<td>0.41</td>
<td>0.51</td>
</tr>
<tr>
<td>3</td>
<td>13.67</td>
<td>489.8</td>
<td>61.44</td>
<td>342.5</td>
<td>0.39</td>
<td>0.99</td>
</tr>
<tr>
<td>4</td>
<td>13.67</td>
<td>402.8</td>
<td>65.64</td>
<td>255.47</td>
<td>0.39</td>
<td>0.99</td>
</tr>
<tr>
<td>5</td>
<td>13.67</td>
<td>184.7</td>
<td>62.64</td>
<td>64.93</td>
<td>0.39</td>
<td>0.99</td>
</tr>
<tr>
<td>6</td>
<td>55.49</td>
<td>205.8</td>
<td>64.6</td>
<td>35.10</td>
<td>0.45</td>
<td>2.36</td>
</tr>
<tr>
<td>7</td>
<td>55.49</td>
<td>156.6</td>
<td>51.2</td>
<td>11.48</td>
<td>0.45</td>
<td>2.36</td>
</tr>
<tr>
<td>8</td>
<td>55.49</td>
<td>485.8</td>
<td>62.3</td>
<td>176.77</td>
<td>0.45</td>
<td>2.36</td>
</tr>
<tr>
<td>9</td>
<td>35.92</td>
<td>301.4</td>
<td>41.8</td>
<td>68.119</td>
<td>0.41</td>
<td>2.94</td>
</tr>
<tr>
<td>10</td>
<td>35.92</td>
<td>487.4</td>
<td>99.8</td>
<td>112.78</td>
<td>0.41</td>
<td>2.94</td>
</tr>
<tr>
<td>11</td>
<td>35.92</td>
<td>207.4</td>
<td>99.8</td>
<td>15.23</td>
<td>0.41</td>
<td>2.94</td>
</tr>
</tbody>
</table>

The results illustrated in Table 5.1 were obtained after performing calibration tests on the metrology measurement tools. In our experimental analysis it was discovered that there was a discrepancy in the readings obtained from the SEM and the optical microscope. For example, for sample 3 in Table 5.1, the length of the cantilever beam was measured to be 488.5 µm by the SEM and 494 µm by the optical microscope. However, this particular beam was designed to be of 497 µm (obtained from the mask file).
Table 5.2 illustrates the above described discrepancy as percentage error computed with respect to the mask values for the length parameter.

Table 5.2: Comparison of Optical microscope and SEM data

<table>
<thead>
<tr>
<th>Sample Number</th>
<th>Percentage error</th>
<th>Optical Microscope</th>
<th>SEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.16</td>
<td>3.6</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>7.3</td>
<td>3.2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td>1.7</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.97</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3.5</td>
<td>3.4</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2.3</td>
<td>5.7</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1.8</td>
<td>6.87</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.4</td>
<td>2.29</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.32</td>
<td>3.88</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.2</td>
<td>3.8</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.92</td>
<td>8.1</td>
<td></td>
</tr>
<tr>
<td>Avg. error</td>
<td>%1.77</td>
<td>%4.04</td>
<td></td>
</tr>
</tbody>
</table>

Analyzing these results, one can conclude that the error in these measurements is either a result of fabrication details or due to the limitations in the metrology tool. The deviation from the actual dimensions of the beams can be minimized to a great extent by exercising accurate control on the process as well as the recipe variables. However, metrology tool limitations are difficult to account for as they are very much dependent upon the resolution and other physical parameters of the tool. Due to these limitations, in our analysis, we choose those values that are near to the mask values. By doing so, it was assumed that that error caused due to the fabrication process is constant in all the test samples.
Figures 5.1 (a) and (b) illustrate the SEM pictures of the some of the released cantilevers discussed in Table 5.1.

Figure 5.1: SEM pictures of the some of the released cantilevers consisting of evaporated aluminum on SiO₂. (a) Side view of the cantilevers obtained with a stage tilt of 81° (b) top view of the cantilevers
In order to study the effects of deposition techniques as well as recipe parameters on the material properties of thin films, another set of bilayer cantilevers consisting of sputtered aluminum and SiO$_2$ were fabricated. In this study, aluminum thin films were sputtered with and without substrate heating. Tables 5.3 and 5.4 illustrate the metrology information of these experiments.

**Table 5.3: Micro-cantilever beams consisting of SiO$_2$ and sputtered aluminum without substrate heating**

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Stress Al (MPa)</th>
<th>$L_B$ (µm)</th>
<th>$W_B$ (µm)</th>
<th>$d_B$ (µm)</th>
<th>Thickness Al (µm)</th>
<th>SiO$_2$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18.8</td>
<td>464.3</td>
<td>58.26</td>
<td>246.8</td>
<td>0.47</td>
<td>1.93</td>
</tr>
<tr>
<td>2</td>
<td>18.8</td>
<td>386.6</td>
<td>59.15</td>
<td>172</td>
<td>0.47</td>
<td>1.93</td>
</tr>
<tr>
<td>3</td>
<td>18.8</td>
<td>195.9</td>
<td>58.64</td>
<td>53.06</td>
<td>0.47</td>
<td>1.93</td>
</tr>
<tr>
<td>4</td>
<td>18.8</td>
<td>467.4</td>
<td>97.4</td>
<td>170</td>
<td>0.47</td>
<td>1.93</td>
</tr>
<tr>
<td>5</td>
<td>18.8</td>
<td>185</td>
<td>55.51</td>
<td>47</td>
<td>0.47</td>
<td>1.93</td>
</tr>
</tbody>
</table>

**Table 5.4: Micro-cantilever beams consisting of SiO$_2$ and sputtered aluminum with substrate heating**

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Stress Al (MPa)</th>
<th>Stress SiO$_2$ (MPa)</th>
<th>$L_B$ (µm)</th>
<th>$W_B$ (µm)</th>
<th>$d_B$ (µm)</th>
<th>Thickness Al (µm)</th>
<th>SiO$_2$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>92.37</td>
<td>37.7</td>
<td>472.1</td>
<td>61.04</td>
<td>129</td>
<td>0.45</td>
<td>1.95</td>
</tr>
<tr>
<td>2</td>
<td>92.37</td>
<td>37.7</td>
<td>389.8</td>
<td>60.46</td>
<td>95</td>
<td>0.45</td>
<td>1.95</td>
</tr>
<tr>
<td>3</td>
<td>92.37</td>
<td>37.7</td>
<td>201.2</td>
<td>61.71</td>
<td>29.50</td>
<td>0.45</td>
<td>1.95</td>
</tr>
</tbody>
</table>
Figures 5.2 (a) and (b) illustrate the SEM pictures of some of the cantilevers illustrated in Tables 5.3 and 5.4.

Figure 5.2: SEM pictures of micro-cantilevers with SiO$_2$ and sputter aluminum. (a) Aluminum deposited without substrate heating, (b) aluminum deposited with substrate heating
The following sub section illustrates the fabrication results for polyimide and SiO₂ cantilevers.

### 5.1.2 Polyimide and SiO₂ bilayer cantilevers

Using the fabrication process described in Chapter 4, bilayer cantilevers consisting of polyimide as the actuating layer and SiO₂ as the base layer were fabricated. Table 5.5 illustrates the metrology as well as the induced stress information for the various test samples fabricated at RIT. In this table the length, width, thickness, and the static deflection are represented by $L_B$, $W_B$, $T_B$, and $d_B$, respectively.

#### Table 5.5: Micro-cantilevers beams consisting of polyimide and SiO₂

<table>
<thead>
<tr>
<th>No.</th>
<th>$d_B$ (µm)</th>
<th>SiO₂ beam (µm)</th>
<th>Polyimide beam (µm)</th>
<th>Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$W_B$ $L_B$ $T_B$</td>
<td>$W_B$ $L_B$ $T_B$</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>5.86</td>
<td>52.84 147.62 1.9492</td>
<td>29.67 136 1.328</td>
<td>12.08</td>
</tr>
<tr>
<td>2</td>
<td>42.68</td>
<td>51.80 350.36 1.9492</td>
<td>30.34 339.63 1.328</td>
<td>12.08</td>
</tr>
<tr>
<td>3</td>
<td>7.137</td>
<td>29.84 136.1 1.9492</td>
<td>7.3 124.83 1.328</td>
<td>12.08</td>
</tr>
<tr>
<td>4</td>
<td>236.4</td>
<td>80.77 403.15 0.9662</td>
<td>61.83 393.68 2.47</td>
<td>9.613</td>
</tr>
<tr>
<td>5</td>
<td>332.6</td>
<td>81.84 498.44 0.9662</td>
<td>61.56 488.3 2.47</td>
<td>9.613</td>
</tr>
<tr>
<td>6</td>
<td>79.03</td>
<td>51.28 197.69 0.9662</td>
<td>30.98 187.54 2.47</td>
<td>9.613</td>
</tr>
<tr>
<td>7</td>
<td>52.13</td>
<td>60.47 161.62 0.9662</td>
<td>40.71 151.74 2.47</td>
<td>9.613</td>
</tr>
<tr>
<td>8</td>
<td>164.9</td>
<td>63.39 310.30 0.9662</td>
<td>40.04 298.63 2.47</td>
<td>9.613</td>
</tr>
<tr>
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<td>47.51 142.57 2.95</td>
<td>27.98 132.8 2.39</td>
<td>7.08</td>
</tr>
<tr>
<td>10</td>
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<td>49.56 287.8 2.95</td>
<td>26.66 276.35 2.39</td>
<td>7.08</td>
</tr>
<tr>
<td>11</td>
<td>45.75</td>
<td>42.17 350.5 2.95</td>
<td>29.15 344 2.39</td>
<td>7.08</td>
</tr>
<tr>
<td>12</td>
<td>49.39</td>
<td>49.70 308.69 2.95</td>
<td>37.31 302.5 2.39</td>
<td>7.08</td>
</tr>
</tbody>
</table>

An examination of the data in Table 5.5 illustrates that the physical dimensions of TEOS and polyimide film are different. This discrepancy is associated to the long SF₆ plasma etches during the release step. Although the polyimide films were protected by a
hard mask, it was found that the SF6 plasma etched the sides of the cantilevers. Figure 5.3 illustrates the SEM pictures of some of the cantilevers listed in Table 5.5.

Figure 5.3: SEM pictures of micro-cantilevers consisting of polyimide and SiO₂. (a) Top view, (b) side view obtained with a stage tilt of 83.9°
The above described experimental data is modeled in Ansys® with the bulk values for the materials. The following section describes the first proposed approach.

### 5.2 Soft computing approach

#### 5.2.1 Comparison of mechanical behavior predicted by the bulk to experimental values

The bilayer cantilevers Tables 5.1, 5.3, 5.4 and 5.5 were modeled in Ansys®. In these simulations the bulk values for Young’s Modulus of aluminum (70 GPa), SiO₂ (73 GPa) and polyimide (3.3 GPa) were used to simulate the cantilevers. These values were obtained from our work as well as the manufacturer [22, 34].

Figure 5.4 illustrates this deflection mismatch between the experimental values to the simulations for evaporated aluminum on SiO₂ cantilevers for the data samples illustrated in Table 5.1.

![Figure 5.4: Comparison of bulk value deflections to experimental values for evaporated aluminum on SiO₂ cantilevers](image)
Figure 5.5 illustrates the deflection mismatch between the experimental values to the simulations for sputtered aluminum (without substrate heating and with substrate heating) films on SiO₂ cantilevers for the data samples illustrated in Table 5.3 and Table 5.4.

Figure 5.5: Comparison of bulk value deflections to experimental values for sputtered aluminum on SiO₂ cantilevers: (a) Without substrate heating (b) With substrate heating
Figure 5.6 illustrates this deflection mismatch for polyimide on SiO₂ cantilevers for the data samples illustrated in Table 5.5.

Figure 5.6: Comparison of bulk value deflections to experimental values for polyimide on SiO₂ cantilevers

These figures clearly illustrate a substantial mismatch between the experimental deflections and the simulation results. This discrepancy is attributed to the values for the material properties used in these simulations. This discussion clearly emphasizes that existing models are incapable of modeling these large deflections and new techniques are needed to predict the mechanical behavior of MEMS structures. The proposed technique incorporates the effect of dimensions as well as fabrication parameters into its model. As a result, it has the ability to predict the effective elastic modulus with greater accuracy.

The following section illustrates the effective Young’s Modulus obtained by various soft computing techniques.
5.2.2 Computation of effective Young’s Modulus using soft computing

The proposed technique estimates the effective Young’s Modulus values for aluminum, SiO₂ and polyimide using experimental data and finite element analysis. Due to the complex relationship between the various governing factors, in this technique empirical models are generated using various non-parametric based algorithms for searching and learning the mechanical behavior of thin films.

In the searching phase, for each data set, the effective values (for each material) are explored such that the experimental deflections match the finite element simulations as described in Chapter 3 and Chapter 4. Two types of search algorithms namely; 2D search and Micro-genetic algorithm (MGA) were studied. The effective material properties developed by these algorithms were learned using empirical learning techniques such as neural networks and 1D Radial Basis Function networks.

The following subsections illustrate the effective material properties for different types of aluminum, SiO₂ and polyimide. Section 5.2.2.1 illustrates the effective values obtained from the analysis of evaporated aluminum on TEOS cantilevers. Section 5.2.2.2 illustrates the effective values obtained for sputtered aluminum on SiO₂ cantilevers. Section 5.2.2.3 illustrates the effective values obtained from the analysis of polyimide on SiO₂ cantilevers. Section 5.2.3 describes the performance of the soft computing techniques and finally section 5.2.4 validates the effective material properties by simulating a novel MEMS mirror in Ansys®.
5.2.2.1 Analysis of evaporated aluminum on SiO₂ cantilevers

Figure 5.7 illustrates the effective Young’s Modulus values as computed by 2D search and MGA technique for evaporated aluminum for the data sets illustrated in Table 5.1.

![Figure 5.7: Effective Young’s Modulus for evaporated aluminum computed by 2D search and micro-genetic algorithms](image)

This figure clearly indicates that the effective values for Young’s Modulus computed by the two algorithms are very similar and almost an order of magnitude lower than the bulk value. A literature survey revealed that the observed Young’s Modulus of aluminum thin films is less than half the bulk value [35]. Uniaxial tension tests of aluminum specimens varying in thickness between 0.11 to 0.65 µm indicated that the Young’s Modulus value clustered between 23 to 38 GPa [35, 36]. Other investigators report Young’s Modulus values of 1 µm aluminum films to be in the range of 16.5 GPa and 24.1 GPa [35].
Recent analysis of free standing aluminum thin films indicated that material properties of aluminum thin films is greatly dependent upon the grain size [36]. Tensile tests of 1 micron evaporated aluminum thin films of varying grain sizes were found to have different Young’s Modulus values. An average grain size of 35 nm resulted in a Young’s Modulus of 24.1 GPa and that of 100 nm was found to have a Young’s Modulus of 16.5 GPa [36]. In this analysis, the proposed soft computing techniques estimate the effective Young’s Modulus to be in the range of 5 GPa to 15 GPa (Figure 5.7). These values are 10-20% lower than the literature values and this discrepancy can be attributed to the varying aluminum grain sizes during the deposition [36]. As described in the fabrication section of Chapter 4, these films were deposited using a CHA Evaporator that uses a manually feed flash source that had an uncontrolled deposition rate. This variation in the grain sizes across the thickness of the aluminum layers could have resulted in thin films with a higher number of dislocations and lower effective Young’s Modulus.

In the case of SiO2 thin films, the effective Young’s Modulus was also computed to be less than half the bulk value. Figure 5.8 illustrates the effective values of SiO2 obtained for the evaporated Al- SiO2 cantilevers using 2D search technique and MGA. Although the effective values for SiO2 varied depending upon the beam dimensions and the induced stress, the average value was calculated to be 18 GPa.

Please note that this study is by far the most recent and only research on analyzing the mechanical properties of TEOS based SiO2 thin films. As a result, these effective values were not compared to any references.
5.2.2.2 Analysis of sputtered aluminum on SiO$_2$ cantilevers

In order to study the effect of process conditions on the material properties, bilayer cantilevers consisting of sputtered aluminum on SiO$_2$ were fabricated. Unlike evaporation, sputtering is a physical vapor deposition technique that involves bombarding a solid surface (in this case aluminum plate was used) by atoms, ions or molecules. The kinetic energy of the impinging particles enables the aluminum atoms to be ejected into the gas phase which are then deposited on the target wafers.

![Figure 5.8: Effective Young’s Modulus for SiO$_2$ as computed by 2D search and micro-genetic algorithms evaporated aluminum on SiO$_2$](image)

Since this deposition technique involves complex interactions between the various atoms, in literature a comprehensive theory is yet to be developed [54]. As a result, many researchers model the electrical and mechanical behavior using empirical techniques [54]. In this research, soft computing techniques were used to compute the effective
Young’s Modulus for aluminum as illustrated in Figure 5.9. Please note that the process conditions were not altered from before for TEOS thin films.

**Figure 5.9: Effective Young’s Modulus for sputtered aluminum without substrate heating as computed by 2D search and micro-genetic algorithms**

Comparing the effective Young’s Modulus values of evaporated aluminum (Figure 5.7) and sputtered aluminum (Figure 5.9), it can be stated that the effective values for the two processes are different from each other but are much less than the bulk value. This analysis indicates that the fabrication process greatly affects the material properties of the thin films and universal models are prone to huge amount of errors.

In addition to these experiments, another set of cantilevers were fabricated with sputtered aluminum on SiO₂ with substrate heating to study the affect of process conditions on effective Young’s Modulus of thin film materials.
In the literature, it has been shown that large grain sizes are observed in thicker films and films that are deposited on heated substrates [54]. Initial deposition temperature plays an important role in the grain size than post deposition annealing in determining the final grain size [54]. The films formed during such a deposition are known to be more uniform. This is because heated substrates provide increased surface mobility during deposition that results in fewer dislocations [54]. As a result these films are expected to have higher Young’s Modulus than the films that are deposited without substrate heating. Figure 5.10 illustrates the effective Young’s Modulus of sputtered aluminum on heated substrate computed by the soft computing techniques. Although a small sample space, Figure 5.10 illustrates the above described behavior.

Figure 5.10: Effective Young’s Modulus for sputtered aluminum with substrate heating as computed by 2D search and micro-genetic algorithms
Besides estimating the effective Young’s Modulus of aluminum thin films, using these cantilevers (sputtered aluminum on SiO₂ cantilevers) effective Young’s Modulus of SiO₂ thin films was computed. Figures 5.11 (a) and (b) illustrate these plots.

Figure 5.11: Effective Young’s Modulus for SiO₂ computed by 2D search and micro-genetic algorithms: (a) without substrate heating, (b) with substrate heating
Figure 5.11 illustrates that the effective Young’s Modulus values for SiO$_2$ are similar to the previous estimates for MGA when compared to 2D search technique. Since the fabrication process for the TEOS layer was not altered, the observed effective values for all the runs should be similar. This argument shows the limitations of some soft computing techniques.

5.2.2.3 Analysis of polyimide on SiO$_2$ cantilevers

Figure 5.12 illustrates the effective values of Young’s Modulus for polyimide computed by the analysis of polyimide- SiO$_2$ cantilevers using 2D search technique for the data sets in Table 5.5.

![Figure 5.12: Effective Young’s Modulus for polyimide computed by 2D search](image)

The above Figure 5.12 indicates that the effective values of the polyimide thin films are not substantially different from the bulk value of cured polyimide given by the
manufacturer. However, one must note the Young’s Modulus values of cured polyimide films are very different from the uncured polyimide and care must be taken in using the appropriate values. Figure 5.13 illustrates the effective Young’s Modulus values of SiO₂ computed by these cantilevers.

![Effective values of polyimide and SiO₂](image)

**Figure 5.13: Effective values of polyimide and SiO₂ computed by the analysis of Polyimide-SiO₂ cantilevers**

A comparison between the effective values of Young’s Modulus of SiO₂ between the various cantilevers specimens in Tables 5.1 and 5.4 illustrates a noticeable pattern. It was found that the effective Young’s modulus of SiO₂ was very similar for beams that are comparable in dimensions and stresses induced. For example, data sample 3 in Table 5.1 is very similar to data sample 5 in Table 5.4 in dimensions as well as stress induced. The effective Young’s Modulus of SiO₂ for both these samples is around 9 GPa. This discovery emphasizes the credibility of the proposed technique.
The following section illustrates the performance comparison of the empirical modeling techniques that learn the mechanical behavior of thin film materials.

### 5.2.3 Empirical modeling techniques

The effective values computed by 2D search and MGA are very comparable. However the time taken to reach to the optimal solution was substantially different between these two techniques. Figure 5.14 illustrates the performance evaluation based on the number of iterations. This plot clearly shows that MGA reached the optimal solution much faster and in less number of iterations when compared to 2D Search technique.

![Figure 5.14: Performance evaluation of the search techniques based on the number of fitness evaluations](image)

The above generated effective values were then learned using 1D-RBF networks as well as neural networks. Among the 11 data sets, using random selection 7 of them were used for training the networks and the rest were used for testing (data set numbers 2,
Figures 5.15 and 5.16 illustrate the percentage mean square error for aluminum and TEOS respectively.

**Figure 5.15: Performance comparison of various learning techniques for predicting the effective Young’s Modulus for aluminum**

**Figure 5.16: Performance comparison of various learning techniques for predicting the effective Young’s Modulus for SiO₂.**
These bar graphs illustrate the performance of four different combinations that are possible with the two search and two learning techniques. A closer look at these plots indicates that 1D-RBF and GA combination results in the lowest MSE. This observation illustrates that 1D-RBF is capable of capturing the behavior with lesser number of data sets when compared to NN. This salient feature of RBF may be advantageous in situations where there is limited amount of fabrication data.

The proposed methodology was also validated by modeling and fabricating a novel MEMS device that is based on a polyimide based thermal actuator. The following section describes the simulation and fabrication results.

5.2.4 Micro-mirror: fabrication and simulation results

The proposed soft computing methodology was validated by modeling and fabricating a novel MEMS device that is based on a polyimide based thermal actuator. The primary advantage of this device is its compatibility with the backend CMOS processing. The device uses a low temperature TEOS oxide deposited through plasma enhanced chemical vapor deposition (PECVD). The manufactured device is an analog switchable cantilever that is thermally actuated. The actuating material is a cured polyimide that expands when heated through an integrated resistive heater. Figure 5.17 illustrates the schematic of the proposed mirror structure.

The fabrication sequence for this device involves four lithography steps. The first step is to deposit a 2 μm thick TEOS oxide which is followed by sputtering 0.15 μm thick Tungsten-Titanium film that is patterned to form resistive heaters. The next step is to fabricate the bond pads and the connecting wires to the heater elements. This is achieved
by depositing and patterning aluminum thin films. Polyimide is then spin-coated, cured, and patterned such that it covers the heaters and also acts a mechanical hinge.

Figure 5.17: A novel Micro-mirror fabricated at SMFL-RIT

A very thin layer (0.15 μm) of TEOS film is deposited to protect the polyimide thin films during the release etch. Finally, using aluminum as a hard mask the cantilever trench is defined and etched in SF6 plasma to release the structure. Figure 5.18 illustrates the final mirror structure.

Using metrology tools such as the optical microscope and optical profilometer, physical dimensions such as the length, width, thickness and the static deflection of the device were computed. The TEOS beams were measured to be 460 micron long, 95 micron wide and 2.5 micron thick and the polyimide was measured to be 100 micron
long, 85 micron wide, and 2 micron thick. The static deflection of the mirror was computed using the optical profilometer.

Figure 5.18: A novel micro-mirror fabricated at RIT: An optical microscope image of the MEMS device

Although Figure 5.19 illustrates that the maximum deflection of the mirrors is only 7.7 \( \mu \text{m} \), a closer look at the graph indicates the inaccurate position of the zero reference line. A more accurate reading of the deflection was obtained using the line scan feature in the optical profilometer and the new value was found to be 12.5 \( \mu \text{m} \).

Figure 5.19: Screen output of the optical profilometer illustrating the static deflection of the micro-mirror
Static two-dimensional Ansys® simulations were performed for this structure using the bulk values and the effective values generated by the proposed methodology for Young’s modulus. Due to the complicated geometric layout in Ansys® the structure was simplified into various rectangles. As a result, a total of six rectangles were obtained with one each for polyimide and tungsten, and four for SiO₂. This is because in addition to the base SiO₂ layer there is a conformally deposited capping SiO₂ layer whose dimensions vary across the structure. Figure 5.20 illustrates a cross-section view of the Ansys® representation of the structure. Due to the variations in the dimensions of the SiO₂ layer at various sections of the structure, the effective values were computed separately for each section. A total of 6344 elements were used to represent the structure with each element spanning 0.075 μm across the thickness.

![Figure 5.20: Cross-sectional view of the Ansys® representation of the various segments of the micro-mirror (not to scale)](image)

The static deflection obtained using the bulk values for SiO₂ (73 GPa), polyimide (3.3 GPa) and tungsten-titanium (360 GPa) was found to be 4.19 μm with an error of
66.48%. The deflection obtained using the effective values for SiO$_2$ was found to be 14.99 \( \mu m \) with an error of 19.92%.

This example clearly illustrates that the proposed technique is not only able to learn the relationship between the various dimensions of the test device (different from the ones used in training) and the fabrication-induced parameters but also is able to predict the effective material properties that enable accurate modeling of other MEMS devices. The accuracy of the effective values may be easily improved by using more samples in the learning phase [33].

As a summary, the first approach computes the effective material properties based on finite element analysis as well as soft computing techniques. The fundamental assumption in this approach is that by learning the mechanical behavior of a large database of test structures, multi dimensional curves are fitted which can then be used to estimate the effective parameter values for the simulation and fabrication of new designs. Thin films of aluminum, TEOS and polyimide are analyzed using various search and learning techniques. The following section illustrates the working of the second approach that is based on theoretical analysis of bilayer cantilevers.

**5.3 Analytical approach**

In this approach the mechanical behavior of the bilayer cantilevers was modeled using existing theoretical concepts. Unlike the first proposed approach, the primary hypothesis of this work is that Young’s Modulus of thin films remains the same as the bulk value. Thus, the transformation strains induced into the films during deposition are assumed to be the reason for large out-of-plane deflections of the cantilevers. Also, the transformation strains are assumed to be very specific to a process and recipe. As a result,
by modeling the transformation strains, the deflections of the cantilevers can be predicted. The mathematical equations that describe this approach were discussed in Chapter 4.5. As a proof of concept, four sets of bilayer cantilevers were fabricated and analyzed using this approach. Table 5.6 illustrates the dimensions of the cantilever beams that were investigated. Please note that most of the beams listed here are from Tables 5.1, and 5.3 through 5.5. They are listed again for the sake of clarity.

Table 5.6: Cantilevers fabricated at RIT that were used to study the analytical approach

<table>
<thead>
<tr>
<th>Sample No</th>
<th>Length (µm)</th>
<th>Width (µm)</th>
<th>Def. (µm)</th>
<th>Thickness(µm)</th>
<th>SiO₂</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaporated aluminum on SiO₂</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>351.36</td>
<td>64.46</td>
<td>171.74</td>
<td>1.82</td>
<td>0.48</td>
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<td>120.76</td>
<td>1.82</td>
<td>0.48</td>
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<td>40.40</td>
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</tr>
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<td>37.01</td>
<td>1.82</td>
<td>0.48</td>
<td></td>
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<tr>
<td>Sputtered aluminum on SiO₂ (without heating)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
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<td>58.26</td>
<td>246.8</td>
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<tr>
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<td>172</td>
<td>1.93</td>
<td>0.47</td>
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<tr>
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<td>195.9</td>
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<td>53.06</td>
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<td></td>
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<tr>
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<td>467.4</td>
<td>97.4</td>
<td>170</td>
<td>1.93</td>
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</tr>
<tr>
<td>5</td>
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<td>55.51</td>
<td>47</td>
<td>1.93</td>
<td>0.47</td>
<td></td>
</tr>
<tr>
<td>Sputtered aluminum on SiO₂ (with heating)</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>0.45</td>
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<tr>
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<td></td>
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<tr>
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<td>236.4</td>
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<td></td>
</tr>
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<td>45.75</td>
<td>2.39</td>
<td>2.95</td>
<td></td>
</tr>
</tbody>
</table>
The first step in this approach was to compute the radius of curvature of the cantilevers. This information was obtained from the side-angled SEM pictures of the cantilevers. In the literature, many researches have used an approximate formula that relates the length of the beam \( l \) and the observed maximum static deflection \( \delta \) to the radius of curvature \( \rho \) as shown in Equation 5.1. However this equation is valid only for \( l \ll \rho \).

\[
\delta = \frac{l^2}{2\rho}
\]  

(5.1)

As a result, in the case of long cantilevers where \( l \approx \rho \) the above assumption is not valid and can lead to inaccurate results. In order to overcome this limitation, a general equation that relates the tip deflection and the length of the cantilever was derived in [53] and is expressed in Equation 5.2.

\[
\delta = \rho \cdot \left( 1 - \cos \left( \frac{l}{\rho} \right) \right)
\]  

(5.2)

Figures 5.21, 5.22, 5.23, and 5.24 illustrate the radius of curvature computed using the approximate formula (Equation 5.1) as well as non-linear curve fitting technique (Appendix A) for the data samples shown in Table 5.6.

These figures clearly indicate that the approximate formula is greatly dependent upon the length of the cantilever and has a lot of scatter over the data set. Alternate techniques such as the curve fitting (linear and non-linear techniques) were implemented [55].
Please refer to Appendix A for the description of the non-linear curve fitting algorithm used in this research.

Figure 5.21: Computation of radius of curvature for evaporated aluminum on SiO₂ cantilevers using different techniques

Figure 5.22: Computation of radius of curvature for sputtered aluminum on SiO₂ cantilevers using different techniques
Figures 5.21 to 5.24 illustrate the results of the non-linear curve fitting algorithm in comparison to the approximate formula.

Figure 5.23: Computation of radius of curvature for sputtered aluminum (with heat) on SiO₂ cantilevers using different techniques

Figure 5.24: Computation of radius of curvature for polyimide on SiO₂ cantilevers using different techniques
A close look at these figures confirms that the non-linear fitting technique provides relatively consistent radii of curvature for the samples. Also the average values for the radius of curvature for the four sets of cantilevers were different from each other. This implies that there are effects of fabrication process on the mechanical behavior of the cantilevers. After computing the radii of curvature with the non-linear fitting technique, the stresses in the thin films as well as the relative transformation strains were computed.

Using the equations 4.27 through 4.30, the stresses in the bilayers were analyzed at various locations. Figures 5.25 to 5.28 illustrate the stresses at the top and bottom of each layer in the four sets of cantilevers. Theoretical analysis indicates that the top layer of aluminum or polyimide films are known be in compression while the bottom of these films are in tension.

![Stress Measurement](image)

Figure 5.25: Stresses computed at various locations for evaporated aluminum on SiO₂ cantilevers
The same behavior is expected for TEOS films as well.

Figure 5.26: Stresses computed at various locations for sputtered aluminum on SiO$_2$ cantilevers

Figure 5.27: Stresses computed at various locations for sputtered aluminum (with heat) on SiO$_2$ cantilevers
These figures (5.25 to 5.28) illustrate the predicted behavior and also give an idea of the amount of stresses that could be present in the thin films. Although the exact stresses at the interface of the two films are very difficult to compute, this analysis gives an approximate value.

![Stress Measurement](image)

In the following analysis, the transformation strains for the four sets are described. These transformation strains are computed using the general formula equation 4.33 that was derived for thin films of arbitrary dimensions as well as using the formula that is based on Stoney’s approximation 4.34.
Figures 5.29 to 5.32 illustrate these results.

**Figure 5.29:** Relative transformation strains for evaporated aluminum on SiO$_2$ cantilevers

**Figure 5.30:** Relative transformation strains for sputtered aluminum on SiO$_2$ cantilevers
These plots evidently indicate that the transformation strains are fabrication process depended as they have different values for various fabrication techniques.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.31.png}
\caption{Relative transformation strains for sputtered aluminum (with heat) on SiO$_2$ cantilevers}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.32.png}
\caption{Relative transformation strains for polyimide on SiO$_2$ cantilevers}
\end{figure}

Although the sample size is very small in these runs, it can be stated that the relative transformation strains are unique to a process as well as a recipe. As a result, this
research claims that by modeling the relative transformation strains using empirical techniques and a large database of experimental data, the mechanical behavior of cantilevers can be predicted. As a proof of concept, the average values for relative transformation strains (RTS) were computed for each set of cantilevers. This resulted in an average value for RTS for each of the four cantilever experiments. Using this average value as the representative of the process, induced strains and the radius of curvature were computed for each data sample. Figures 5.33 to 5.36 illustrate the deflections computed by the general formula as well as Stoney’s approximation. In these figures, Predicted 1 refers to $\Delta \varepsilon^T$ from the general formula and $Tip_{def} = \frac{12}{2\rho}$, Predicted 2 refers to $\Delta \varepsilon^T$ from the general formula and $Tip_{def} = \rho \left(1 - \cos \left(\frac{1}{\rho}\right)\right)$, Predicted 3 refers to $\Delta \varepsilon^T$ from the Stoney’s formula and $Tip_{def} = \frac{12}{2\rho}$, and Predicted 4 refers to $\Delta \varepsilon^T$ from the Stoney’s formula and $Tip_{def} = \rho \left(1 - \cos \left(\frac{1}{\rho}\right)\right)$.

![Tip deflections](image)

**Figure 5.33:** Tip deflections computed for evaporated aluminum on SiO$_2$ using different techniques
In these plots the tip deflection was computed using the approximate formula (equation 5.1) as well as the general formula (equation 5.2).

Figure 5.34: Tip deflections computed for sputtered aluminum on SiO₂ using different techniques

Figure 5.35: Tip deflections computed for sputtered aluminum (with heat) on SiO₂ using different techniques
Analysis of the tip deflection plots (figures 5.33 to 5.36) indicates that the average value for the relative transformation strains can predict the mechanical behavior of shorter beams to a great accuracy but fail to predict the mechanical behavior of longer beams.

![Tip Deflection Chart](image)

**Figure 5.36: Tip deflections computed for polyimide on SiO₂ using different techniques**

Also, the tip deflection computed using the general equation for the radius of curvature has smaller errors when compared to the corresponding approximate formula for longer beams. This discovery justifies the use of general formula for long cantilevers.

In summary this approach is based on developing mathematical models using theoretical concepts. As a result, this technique does not require finite element analysis. This, by far, is the greatest advantage of this technique. However, it can not be generalized for other structures as a complete redo of the mathematical analysis is necessary for a different structure. The first approach is more general technique which could be applied to different structures as long as a feedback parameter can be measured for learning and modeling.
Apart from introducing the concept of effective material properties, this research introduces a quantity called confidence factor that quantifies the accuracy of the material properties as well as the simulation results. This factor is developed using fuzzy logic. The following section describes the working of this concept.

5.4 STEAM: Confidence factor

Due to the complex relationship between the fabrication techniques and the fabrication-induced parameters with the metrology of the test structure, mechanical behavior models of thin films are still at their infancy. As a result, to minimize design errors, a confidence factor is needed that validates the estimates done by the empirical models. In the proposed technique this factor is modeled using the concepts of fuzzy logic.

As described in Chapter 3, the input variables of the fuzzy confidence system are the fabrication facility, the complement of mean square error and number of datasets. The output of the system is the confidence factor given as a percentage value. This factor is modeled using various combinations of the input membership functions. The working of this technique is illustrated by computing the confidence factor of effective Young’s Modulus for evaporated aluminum thin films. The following subsection is organized as follows. Section 5.4.1 describes the fuzzy rules that were developed for this system. This was done by using the “rule viewer” module of the fuzzy toolbox in Matlab®. Finally, Section 5.4.2 validates performance of the fuzzy confidence factor.
5.4.1 Fuzzy rule base systems

Since the variation of the material properties across fabrication facilities cannot be quantized mathematically, fuzzy IF-THEN rules are used to model the mechanical behavior [54]. Fuzzy IF-THEN rules are conditional statements that play a key role in representing expert knowledge and linking the input and output variables. In this analysis, fuzzy rules were developed with the help of information obtained from expert users [54]. Table 5.7 illustrates the some of the questions and answers that were used to design the rules.

The questions in this table refer to the expected variation of the material properties for different cases with respect to the input variable, fabfacility. For example, as shown in Table 5.7, a material fabricated in the same fabrication facility using the same tool and same recipe should show a “little” variation in its properties. This behavior was captured in the following fuzzy rule

“If (fabfacility is SPSTSR) and (CMSE is VHIGH) and (datasets is LARGE) then (Value is VLARGE)”

The proposed fuzzy system consists of 18 rules that relate the three input variables and one output variable. The designing of the rules as well as the fuzzy system is a one-time process (that can be altered if necessary). In this analysis the fuzzy system was designed to have a Mamdani inference system [42]. This inference system is used in a fuzzy rule to determine the rule outcome from the given rule input formation. It represents the “THEN” part of the fuzzy rule. The other fuzzy parameters are defined as follows: the “and” operation was defined as minimum, implication was defined as
minimum, *aggregation* was defined as maximum and finally *defuzzification* was defined to be centroid process.

Table 5.7: Information obtained from the expert user for designing the fuzzy rules [56]

<table>
<thead>
<tr>
<th>Questions</th>
<th>Expected variation in material properties</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Little</td>
</tr>
<tr>
<td>1) The same recipe is used in the same tool in the same plant is used?</td>
<td></td>
</tr>
<tr>
<td>2) A different recipe is used in the same tool in the same plant is used?</td>
<td></td>
</tr>
<tr>
<td>3) A different tool in the same plant with same principle of deposition (example, CHA Evaporator vs CVC Evaporator) is used?</td>
<td>X</td>
</tr>
<tr>
<td>4) A different tool in the same plant with different principle of deposition (example, Oxide growth vs Oxide Deposition) is used?</td>
<td></td>
</tr>
<tr>
<td>5) The same tool (same make and model), same recipe, in a different plant is used?</td>
<td></td>
</tr>
<tr>
<td>6) A different recipe in the same tool (same make and model) in a different plant is used?</td>
<td></td>
</tr>
<tr>
<td>7) A different tool, in a different plant with the same principle of deposition is used?</td>
<td></td>
</tr>
<tr>
<td>8) A different tool in a different plant with the different principle of deposition?</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5.37 illustrates the snapshot of the “rule viewer”, a feature of the Matlab® fuzzy toolbox.

5.4.2 Validation of the fuzzy system

The fuzzy system was validated by estimating the effective values of evaporated aluminum thin films. The sample under study belonged to the “same tool, same recipe” category of the fuzzy input variable fabfacility. The empirical model that was used has a CMSE of 0.83 (2Dsearch and RBF combination) with a training set that had large set of...
data points to learn the behavior. The sample that fits the above description is sample 6 in Table 5.1 (evaporated aluminum on TEOS). This is an ideal test sample as it was not used for training the RBF.

The above fuzzy input information was fed to the fuzzy system and the confidence factor was found to be 85%. A quick comparison was performed between the actual and the predicted (using RBF network) effective Young’s Modulus of this sample. It was found that the actual effective Young’s Modulus value was 1.5 GPa and the predicted Young’s Modulus value to be 1.8 GPa (error of 16.67%).

The above discussion thus validates the fuzzy confidence factor as it is able to estimate the error in the prediction made by the empirical models. As a result this tool is envisioned to be a great resource to MEMS engineers as it quantifies the accuracy of the predicted results before physical prototyping.

The following chapter provides the conclusions and future work by highlighting the salient features of this research work. Special emphasis is on possible extensions that can be pursued in the lines of this thesis with a goal of developing a software framework that enables accurate simulations of MEMS devices.
Chapter 6: Conclusions and Future work

The lack of proper mechanical behavior models for thin films has significantly limited the growth and commercialization of MEMS devices. With this as the motivation, the following contributions have been made in this research work:

- A generalized methodology was developed to compute the mechanical properties of thin films. The proposed architecture emphasizes modeling the mechanical behavior of standard test structures through empirical analysis of experimental data. Models developed for these test structures are then utilized for predicting the behavior of structures with arbitrary dimensions.

- Realizing the fact that the mechanical properties of the same thin film material deposited in two fabrication facilities can differ substantially, a Software Tool based on Empirical Analysis of MEMS (STEAM) has developed to model mechanical properties of thin films with respect to the tools and recipes in a given fabrication facility.

- A novel fuzzy confidence factor was developed in STEAM that validates the mechanical properties predicted by the empirical methods. This parameter provides the MEMS designer with a percentage error in the predictions as a measure of confidence in the new design.

- The proposed methodology is comprised of two approaches namely soft computing and analytical approaches that can be used for modeling the mechanical behavior of thin films.
• In the soft computing approach, the mechanical behavior of the thin films is estimated and predicted with the help of various soft computing algorithms such as genetic algorithms, neural networks, radial basis functions network, and search techniques. By using these “intelligent” techniques, the relationship between the various factors that affect the material property can be learned such that reliable predictions can be made. As a result, this technique is very useful in modeling scenarios where the understanding of the exact physics is very limited. Also, due to the built-in generalization, the empirical models developed by these techniques can be used for predicting the mechanical behavior of arbitrary dimensions.

• On the other hand, an analytical approach relies on existing theoretical concepts to analyze the mechanical behavior of thin films. Hence this technique can compute the mechanical behavior without the use of finite element analysis. However, this technique can only model the mechanical behavior of the device under consideration, and generalization to other structures may not be possible.

• The working of the proposed technique was tested by analyzing the Young’s Modulus of thin films. Micromachined bilayer cantilevers were used as test structures. Bilayer cantilevers of various dimensions were fabricated and analyzed to extract mechanical models for three thin film materials: Aluminum, TetraEthylOrthoSilicate (TEOS) based SiO₂, and Polyimide.

• In the analysis of mechanical behavior of the bilayer cantilevers using the soft computing techniques, the fabrication uncertainty was modeled in the Young’s Modulus of the thin film, thus resulting in effective Young’s Modulus values. The various algorithms that were implemented during the estimation phase were 2D
search technique and Micro-Genetic algorithms. In the prediction phase Neural Networks and Radial Basis Function Networks were implemented. Analysis of the generated effective Young’s Modulus values revealed that the performance of the soft computing is superior to the existing methods. In addition, the effective values generated using this methodology are comparable to the values reported in the literature. Given a finite number of data samples, the combination of 1D-RBFN (prediction phase) and GA (estimation phase) presented the best results.

- The generated effective values were also tested by designing and fabricating a novel analog switchable MEMS mirror. It was found that the mechanical response predicted by the effective values had an error of 19% as opposed to 66% when simulated using bulk material properties. This clearly indicates the generalization abilities of the soft computing techniques.

- In the analysis of the mechanical behavior of the cantilevers using the analytical approach, the Young’s Modulus of the materials was assumed constant and the fabrication uncertainties were modeled in the relative transformation strains (RTS). A detailed analysis was performed in which it was found that the RTS values were process-and recipe-dependent.

The following are possible extensions and future work that are envisioned for this work:

- The proposed methodology can be easily utilized to study other material properties of thin films such as coefficient of thermal expansion. The test structure illustrated in [57] can be used to extract this parameter. Due to the lack
of proper understanding of the physics in this structure, a soft computing approach should be utilized to generate reliable models.

- Among the various features of the proposed simulation tool, the most important is the Matlab® to Ansys® interface. However, in the present setup, the graphical User Interface (GUI) permits the users to apply structural loading. This feature can be easily extended to other energy domains such as thermal, electrical, etc. This additional feature would strengthen the user interface, thereby making the software more user-friendly.

- In the soft computing approach, apart from the four tested algorithms, alternative search and learning techniques such as support vector machines, Bayesian networks, etc. can be implemented. As long as these algorithms are implemented in Matlab®, they can be integrated into STEAM directly.

- Finally, a detailed study is warranted for the analysis of relative transformation strains. Studying the RTS values over a wide range of test samples might result in a relationship between the physical dimensions of the device and the RTS values for a particular recipe/tool. Thus by modeling this relationship, predictive capability can be achieved.
Appendix A: Computation of Radius of Curvature

In the analytical approach presented in this research work, the radius of curvature of the self-deformed cantilevers was computed using an iterative non-linear curve fitting algorithm that was based on least squares technique [55]. The following discussion illustrates the working of this technique as applied in this research. Reference [55] may be consulted for more information about the algorithm.

The first step in the process was to obtain raw two-dimensional data points that represent the self-deformed cantilevers. This information was extracted from the side-angle view SEM pictures of the cantilevers. Depending upon the length of the cantilever, an average of 30 coordinates were noted for each cantilever. Using the linear curve fitting algorithm, approximate values for center and radius of the circle that needs to be fitted were computed. These estimates were used as an initial guesses for the solution and an iterative non-linear fitting technique was used to compute the actual values for the center and radius of the fitted circle.

As an example, let us consider the first data set in Table 5.3. This bilayer cantilever consists of sputtered aluminum on TEOS and is 464.4 µm long, 58.26 µm wide with aluminum thickness of 0.47 µm and TEOS thickness of 1.93 µm. The tip deflection was computed to be 246.8 µm. Figure A1.1 illustrates the side-angle view of this cantilever. Thirty seven (37) two-dimensional coordinates were extracted from Figure A1.1 that represent the out-of-plane deflection of the cantilever. With the help of a linear curve fitting technique, the 37 data points were analyzed to compute the initial guesses
for the center and radius of the fitted circle. The following equations represent the mathematical equations that were used in this process.

Let \( (x_o, y_o) \) be the center of the circle and \( r_{\text{linear}} \) be the radius of the curvature obtained using the linear curve fitting algorithm of the circle represented in Equation A.1.

\[
A \cdot (x^2 + y^2) + B \cdot x + C \cdot y = 1
\]  

(A.1)

Equation A.1 can then be solved to find the center and radius as follows.

\[
x_o = \frac{-B}{2A}, \quad y_o = \frac{-C}{2A} \quad \text{and} \quad r_{\text{linear}} = \frac{\sqrt{4 \cdot A + B^2 + C^2}}{2A}
\]  

(A.2)

Where \( A, B, C \) can be computed by solving the matrix in Equation A.3.
The above analysis gives us an initial guess of the solution. This information is then analyzed using an iterative non-linear technique to compute the actual values. Equation A.4 shows an alternate representation of the circle.

\[
\sqrt{(x_i - x_o)^2 + (y_i - y_o)^2} - r = 0
\] (A.4)

The Jacobian matrix, \( J \) for Equation A.4 can then be expressed by Equation A.5.

\[
J = \begin{bmatrix}
\frac{\partial F_1}{\partial x_o} & \frac{\partial F_1}{\partial y_o} & \frac{\partial F_1}{\partial r} \\
\frac{\partial F_2}{\partial x_o} & \frac{\partial F_2}{\partial y_o} & \frac{\partial F_2}{\partial r} \\
\vdots & \vdots & \vdots
\end{bmatrix}
\] (A.5)

Where

\[
\frac{\partial F_1}{x_o} = \frac{x_o - x_i}{\sqrt{x_i^2 - 2 \cdot x_o \cdot x_i + y_i^2 - 2 \cdot y_o \cdot y_i + x_o^2 + y_o^2}}
\] (A.6)

\[
\frac{\partial F_1}{y_o} = \frac{y_o - y_i}{\sqrt{x_i^2 - 2 \cdot x_o \cdot x_i + y_i^2 - 2 \cdot y_o \cdot y_i + x_o^2 + y_o^2}}
\] (A.7)

\[
\frac{\partial F_1}{r} = -1
\] (A.8)

The next step involves the computation of the residual matrix \( K \), given by equation A.9.

\[
K = \begin{bmatrix}
1 \quad \frac{\sqrt{(x_1 - x_o)^2 + (y_1 - y_o)^2} - r}{0} \\
\vdots
\end{bmatrix}
\] (A.9)
Since the cantilever is represented with 37 data points, the size of the $J$ matrix is $(37 \times 3)$ and $K$ matrix is $(37 \times 1)$. Let the delta adjustments on the center and radius values be mathematically represented as in Equation A.10.

$$\Delta X = \begin{bmatrix} \Delta x_o \\ \Delta y_o \\ \Delta r \end{bmatrix}$$  \hspace{1cm} (A.10)

Then the adjustments on the unknowns can be computed using Equation A.11.

$$\Delta X = \left( J^T J \right)^{-1} J^T K$$  \hspace{1cm} (A.11)

Finally, the circle parameters are adjusted using the Equation A.12 until the mean of the adjustments fall below a tolerance of 0.001.

$$x'_o = x_o + \Delta x_o, \quad y'_o = y_o + \Delta y_o, \quad r' = r + \Delta r_o$$ \hspace{1cm} (A.12)

Figure A1.2 illustrates the fitted circle on the 37 data points that represent the cantilever.

Figure A1.2 Illustration of the working of the non-linear curve fitting technique for a cantilever.
The above analysis results in a radius of curvature of 479.55 µm for the cantilever under consideration. This value is very different from the value obtained using the approximate formula, which is 436.73 µm.

In summary, this section illustrates an alternative technique for computing the radius of curvature of cantilevers that are deflected out-of-plane.
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