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Application of Soft Computing Techniques to Estimate the Effective Young's Modulus of Thin Film Materials

Ajay Pasupuleti and Ferat Sahin

***Abstract*— This research aims at characterizing and predicting the Young's Modulus of thin film materials that are utilized in Microelectromechanical systems (MEMS). Recent studies indicate that the mechanical properties such as Young's Modulus of thin films are significantly different from the bulk values. Due to the lack of proper understanding of the physics in the micro-scale domain the state-of-art estimation techniques are unreliable and often unfit for use for predicating the mechanical behavior of slight modifications of existing designs as well as new designs. This disadvantage limits the MEMS designers to physical prototyping which is cost ineffective and time consuming. As a result there is an immediate need for alternative techniques that can learn the complex relationship between the various parameters and predict the effective Young's Modulus of the thin films materials. The proposed technique attempts to solve this problem using empirical estimation techniques that utilize soft computing techniques for the estimation as well as the prediction of the effective Young's Modulus. As a proof of concept, effective Young's Modulus of Aluminum and TetrathylOrthoSilicate (TEOS) thin films were computed by fabricating and analyzing self-deformed micromachined bilayer cantilevers. In the estimation phase, 2D search and micro Genetic algorithm were studied and in the prediction phase, back propagation based Neural networks and One Dimensional Radial Basis Function Networks (1D-RBFN) were studied. The performance of all combinations of these soft computing techniques is studied. Based on the results, we conclude that performance of the soft computing techniques is superior to the existing methods. In addition, the effective values generated using this methodology is 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. Due to these advantages, this methodology is foreseen to be an essential tool for developing accurate models that can estimate the mechanical behavior of thin films.**

***Index Terms*— MicroGenetic algorithm, Radial Basis Function networks, Thin films and Young's Modulus.**

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A. Pasupuleti is pursuing his PhD in Microsystems at Rochester Institute of Technology, Rochester, NY 14623 USA (Phone: 585-475-7208; fax: 585-475-2175; e-mail: axp1014@ rit.edu).

F. Sahin, is the Associate Professor in Electrical Engineering at Rochester Institute of Technology, Rochester, NY 14623 USA. (E-mail: feseee@rit.edu).

I. Introduction

In the last decade materials such as glass, silicon, nitride, and metals were used extensively as structural components in the microscale domain to form microelectomechanical systems (MEMS). These small devices have found their applications in a wide range of areas such as microelectronics, magnetic, optical, electrochemical, and biological technologies [1-5]. This rapid expansion is due to recent advancements in the engineering sciences especially in the area of thin film materials that range from a few angstroms to a few microns in thickness.

Due to wide spread applications of MEMS devices emphasis was on improving device behavior models for performance enhancement and long term reliability [4, 5]. 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 [6-10]. This discrepancy is associated with the scaling effects and the thin-film deposition processes [6-10]. As the size of the MEMS device is reduced, the effect of the dimensions on the mechanical properties becomes more predominant. As a result, the material properties are found to deviate significantly from the bulk scaling laws [7]. On the other hand, deposition techniques greatly influence the material properties such as residual stresses and the elastic modulus induced into the thin films. Examples of some of the process variables that are very specific to the deposition tool that influence the material properties of thin films are substrate temperature, working gas species and their pressure, and orientation of the deposition surface relative to the direction of coating [10].

This research aims at characterizing and predicting the Young's Modulus of thin film materials using soft computing techniques. Among the various mechanical properties, emphasis has been on understanding the Young's Modulus of thin film materials [6- 10]. This is due to the fact that several design issues such as resonant frequency, stiffness, as well as the accuracy of the finite element analysis are greatly affected by this parameter [8]. Tensile test of free standing aluminum thin films of thicknesses ranging from 0.11μm to 1μm indicate that the observed values for Young's Modulus are clustered between 16.5 GPa to 49 GPa [11]. These values are much lower than the bulk value, 70 GPa. Although the reason for this drop has not been completely understood yet, it is often associated to factors such as differences in grain sizes and grain orientation, and small thicknesses of thin films [11, 12]. This discussion illustrates that any generalization of the Young's Modulus on the basis of geometry, deposition technique and thin film structure could result in inaccurate modeling.

In literature, various techniques were developed to characterize the Young's Modulus of thin film materials. These techniques employ nanoindentation [13], changes in natural frequency [14], evaluation of the deflection of buckled membranes [15], as well as membrane deflection under uniform pressure [16]. Unfortunately all these techniques require complicated experimental setup. In some cases mechanical contact between the probe and micromachined structures is inevitable during measurement [7]. These disadvantages may lead to undesired effects during measurement that might lead to very low signal to noise ratio making the data unfit for characterization [7]. As a result, there is a need for indirect measurement techniques that are simple to implement as well as determine the Young's Modulus of thin films by studying the intrinsic properties of the thin films [7]. Literature reveals self deformed micromachined bilayer cantilevers to be ideally suited for such purposes [7, 8]. This is because micromachined cantilevers are often subjected to residual stresses during the deposition process that results in an out-of-plane deflection of the free end of the cantilever [7]. However, given the complexity in the relationship between the device dimensions and fabrication associated parameters, many researchers are looking at analytical solutions that can learn and predict this behavior [17-19]. Among the various techniques, empirical estimation techniques that are based on non-parametric algorithms have been proved to be the most effective [18]. This is because these techniques are able to relate the loading parameters, material properties, fabrication induced parameters, and geometry of the microstructures with their performance characteristics with great accuracy [18].

In this research, micromachined bilayer cantilevers consisting of aluminum and TetraEthylOrthoSilicate (TEOS) have been analyzed. In the process, Young's Modulus was estimated using various techniques such as 2D search, micro-genetic algorithms (MGA), neural networks (NN) and radial basis functions (RBF). The developed models were tested with experimentally obtained data and the results were found to be very encouraging.

The paper is organized as follows. In section 2 the proposed methodology is described. This section also illustrates the implementation of 2D search, MGA, NN and RBF for estimating the effective Young's Modulus of thin films. Section 3 illustrates the performance of the proposed technique which is followed by conclusions and future work in Section 4.

II. Proposed Technique

As discussed in the previous section, mechanical behavior models for thin film materials are still at their infancy. To this effect, an alternative approach was proposed [18]. Figure 1 illustrates the working of the proposed methodology. This methodology involves mathematical modeling, fabrication, ANSYS modeling and empirical estimation.

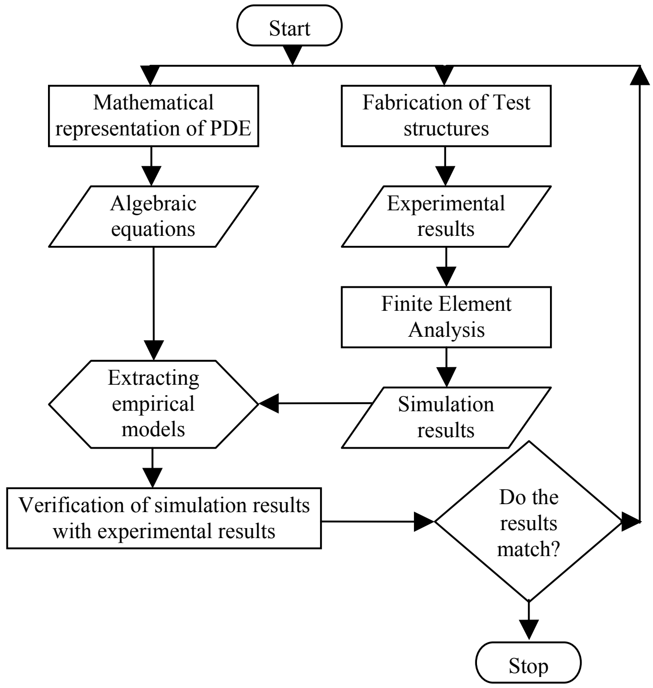


Figure 1: Flow chart of the proposed technique [18]

The first step in this method is to identify the physical phenomena and the boundary conditions that define microcantilevers. This information is then used for extracting the relationship between the governing factors as well as for the design of the fabrication process. Experimental results are obtained by fabricating microcantilevers of various dimensions. Finite element analysis (FEA) is performed on this experimental data and effective material properties are computed. Empirical models are then extracted by correlating the algebraic equations and the FEA results for a large number of data sets. Please refer to our previous work for more information [18-19].

The following sections describe the mathematical modeling, ANSYS® modeling which generates the effective Young's Modulus as well as the various empirical model extraction techniques that could be used for this application.

A. *Mathematical representation*

This investigation contains a general theory of bending of a bilayer cantilever subjected to uniform residual stresses. Figure 2 illustrates a schematic of a typical bilayer cantilever. 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:

$$P_1 = P_2 = P \text{ and} \tag{1}$$

$$\frac{P \cdot h}{2} = M_1 + M_2 \tag{2}$$

Applying the concepts of flexure rigidity from Beam Theory [7] we can express the above equation as follows.

$$\frac{P \cdot h}{2} = \frac{E_1 \cdot I_1 + E_2 \cdot I_2}{\rho} \tag{3}$$

where ρ 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 given by $a_1 + a_2$. Assuming that the stress is uniform, we can express stress (σ) in terms of force (P) and cross sectional area (A).

$$\sigma = \frac{P}{A} \tag{4}$$

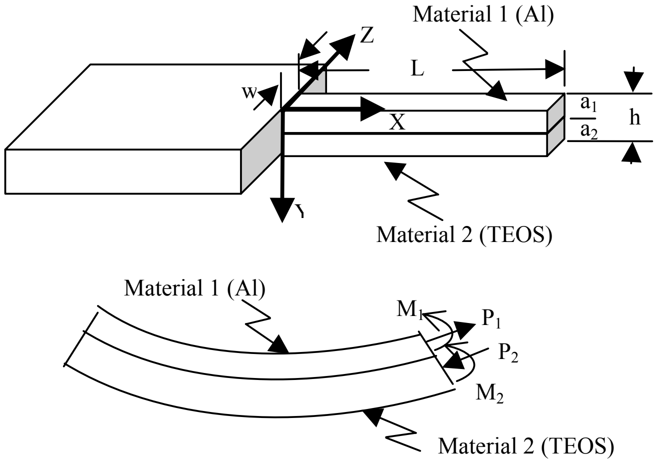


Figure 2: Schematic of bilayer cantilevers

Moment of inertia, I , for each layer is expressed given by the following equation (5).

$$I_1 = \frac{w \cdot a_1^3}{12}, I_2 = \frac{w \cdot a_2^3}{12} \tag{5}$$

Also using Beam Theory [7], one can compute the maximum static deflection (δ) for a beam clamped at one end, which is expressed as follows.

$$\delta = \frac{l^2}{2\rho} \tag{6}$$

Substituting equations (4), and (6) in (3) and simplifying the equation, the following resultant equation is obtained

$$\frac{\sigma \cdot h \cdot (h \cdot w)}{2} = \frac{E_1 \cdot I_1 + E_2 \cdot I_2}{\frac{l^2}{2\delta}} \tag{7}$$

Which can be further simplified to result in (8).

$$\frac{\sigma \cdot h^2 \cdot l^2 \cdot w}{4 \cdot \delta} = E_1 \cdot I_1 + E_2 \cdot I_2 \tag{8}$$

Now substituting equation (5) in (8) and using $h = a_1 + a_2$, the above equation can be further simplified to

$$\frac{3 \cdot \sigma \cdot (a_1 + a_2)^2 \cdot l^2}{\delta} = E_1 \cdot a_1^3 + E_2 \cdot a_2^3 \tag{9}$$

Assuming that the terms in equation (9) can be decoupled, we can extract the relationship of the elastic modulus with the other quantities. Thus the proportionality equation is expressed as follows.

$$E \propto (\sigma, l, a, \delta) \tag{10}$$

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 many researchers [6]. Experimental analysis of bilayer cantilevers of various dimensions illustrate that the width of the cantilever clearly affects the Young's Modulus of thin films [6]. This is because the stresses induced in the cantilever (see Figure 2) 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 [6]. As a result, in the proposed methodology, the width of the cantilevers is taken into account to in estimating the Young's Modulus. Also, as discussed before residual stresses induced into the materials are to a large extent dependent upon the process variables. Thus, the relationship in the equation (10) is nonlinear and can only be estimated empirically. Hence the effective elastic modulus can be expressed as a function of the beam dimensions as well as the stress induced into the bilayer cantilevers during the fabrication process as illustrated in equation (11).

$$\hat{E} = f(\sigma, w, l, a, \delta) \tag{11}$$

Thus the above equation illustrates the relationship between the material property under consideration and the physical parameters. This relation forms the basis for data collection as well as the model generation algorithms.

B. Finite Element modeling and search techniques

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 TEOS for each data set obtained from the fabrication results. These values were computed by modifying the bulk values until the simulations matched the experimental results. A literature survey as well as previous simulation results obtained by the authors indicated that the search space was material dependent [18]. It was found that aluminum varied between 2 GPa to 70 GPa (bulk value) and TEOS varied between 10GPa to 73GPa [11, 18]. Due to this wide spread in the search space, intelligent search techniques are desired for faster results and better accuracy. In this analysis, two types of search techniques viz. two dimensional gradient search technique and micro-genetic algorithms were analyzed and their performance was compared. The following sub-section describes these two algorithms briefly.

1) Two dimensional gradient search technique

This search technique is commonly used in optimization problems where the solutions cannot be obtained using analytical methods [20]. In this technique, the effective Young's modulus of the material is computed using an iterative gradient descent vector that determines the step size as well as direction of the movement. The following equations describe this behavior mathematically.

$$E^1_{eff,itr} = E^1_{eff,itr-1} \pm \nabla E^1_{const} \times E^1_{eff,itr-1} \quad (12)$$

$$E^2_{eff,itr} = E^2_{eff,itr-1} \pm \nabla E^2_{const} \times E^2_{eff,itr-1} \quad (13)$$

where $E^1_{eff,itr}$ and $E^2_{eff,itr}$ represent the current effective Young's modulus for the top layer material and the base layer material, respectively. The symbols ∇E^1_{const} and ∇E^2_{const} are the constant gradients given as 0.7 and 0.12 for material "1"and material "2" respectively.

Figure 3 is a pictorial representation of the working of 2D search technique in computing the effective values of Young's Modulus.

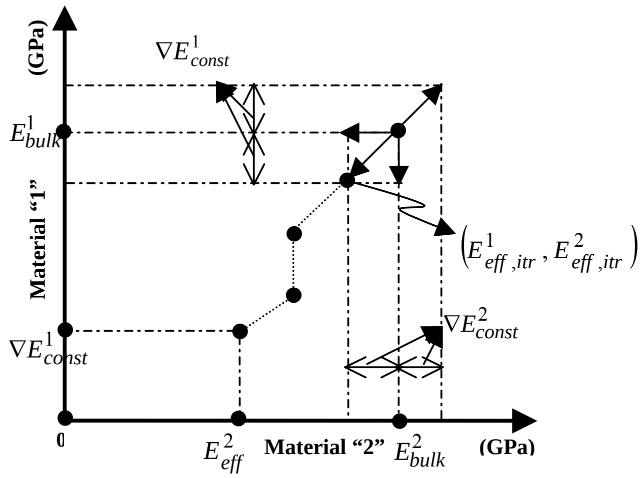


Figure 2: Implementation of 2D Search technique

The algorithm starts with the use Bulk values for materials as initial values. In every epoch, four combinations of effective values are computed and their corresponding deflections are determined using a MATLAB and ANSYS interface [19]. These deflections are ranked based on the error and the combination that results in the least error is used for the next iteration. The process is repeated until the error is less than a tolerance value of 5%.

2) Micro-genetic Algorithm (MGA)

Another popular non-linear search technique is the genetic algorithm [21]. In this technique Young's modulus is quantified into 32 levels. Each element of the Young's Modulus is treated as a gene and a standard GA procedure is applied optimally to select crossover and mutation functions [21]. 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 [21-22].

A modification of this technique is the micro-genetic algorithm [22]. In MGA, only five parents are used in any generation and the successive generations are computed with the crossover of two parents. Figure 4 illustrates the crossover and new parent formation in MGA. The crossover and mutation algorithms used in MGA are similar to the corresponding GA application. The stopping criteria used in this algorithm is the mean square error with a tolerance of 5%.

(12)

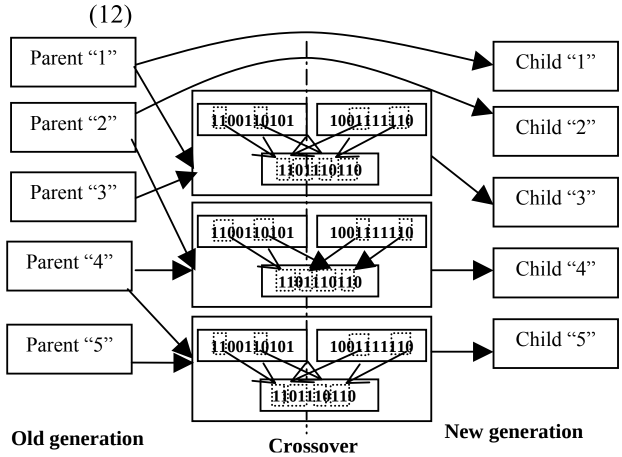


Figure 4: Implementation of MicroGenetic Algorithm (MGA)

C. Empirical Estimation Technique

As discussed in previous sections, 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. In literature various techniques have been reported for predicting as well as learning the behavior of complex relationships between the design variables [20-24]. Among the various factors that affect the choice of the algorithms is the amount of training data available and the number of design variables.

The available algorithms can be broadly classified as parametric and non-parametric based algorithms. In the 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 the maximum likelihood estimation, Bayesian estimation method and standard regression techniques [20]. 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 by the non-parametric methods were the primary assumption is that similar inputs have similar outputs [20]. As a result the emphasis is in modeling the similarities in the data. Also in this technique available data is classified into training set and testing vectors. By doing so, the performance of the learning algorithm can be easily monitored. Most learning algorithms such as RBF and Neural networks fall in this category. In this research these two techniques were analyzed and their performance was compared.

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 [20, 23]. 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 viz. 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 14 and 15 illustrate the mathematical representation of the hidden nodes and the output nodes.

$$h(m) = sigmoid(\sum_{i=1}^{4} x_i w_{i,m}) \quad (14)$$

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

$$\hat{E}(m) = sigmoid(\sum_{i=1}^{6} \sum_{j=1}^{5} h_{i,j} w_{i,j,m}) \quad (15)$$

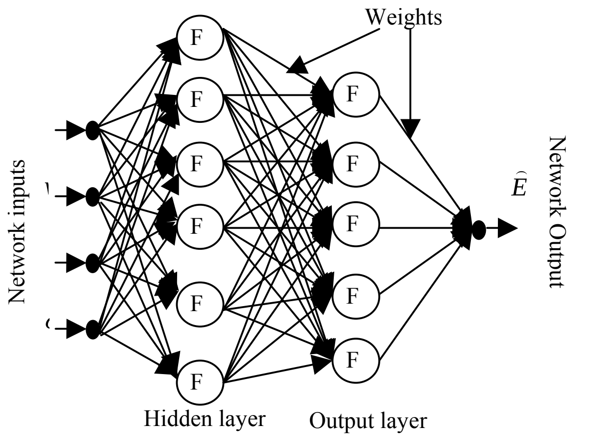


Figure 5: Architecture of the back propagation based neural networks

The most popular technique that is used for training these networks is the back propagation algorithm [23]. The physical dimensions of the beams as well as the fabrication induced parameters are fed as the input to the network. The weights of the network are iteratively adjusted such that the output of the network tracks the effective Young's Modulus values. As this technique uses gradient descent for updating the weights, it is simple and easy to use. However, it is susceptible to long training times [23].

2) One-dimensional Radial basis networks

In the literature, for empirical models in multi-dimensional space, RBF networks are the most popular [23, 24]. 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 [24]. The 1D-RBF networks consist of three layers viz. input layer, hidden layer, and the output layer. The input layer consists of four elements which are stress, length, width, and thickness of the beam. The output of the network is the estimated Young's Modulus ($\hat{E}$).

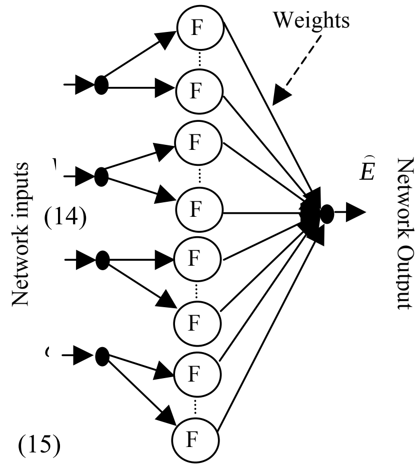


Figure 6: Architecture of 1D- Radial Basis Function Networks

The outputs of the hidden RBFs' used in this network are Gaussian in form and are given by equation (16).

$$F_{k+(p-1)M} = \exp\left(-\left(x_p - c_{pk}\right)^2 / \sigma_{pk}^2\right), \ k = 1,2,....M \quad (16)$$

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 σ_{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.

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

where D_{out} is the desired output which is the ANSYS® estimate of the Young's Modulus.

III. RESULTS

In this section experimental data obtained by fabricating bilayer cantilevers is analyzed. The effective Young's Modulus of thin films is estimated using the combination of search and learning techniques described previous. The performance of these soft computing techniques is evaluated under various scenarios.

A. Fabrication

Bilayer cantilever beams comprising of aluminum on TEOS were fabricated at SMFL [24]. The fabrication process involved two deposition steps (for TEOS and aluminum) and one photo lithography step which was used to pattern the cantilever beams. Metrology tools such as scanning electron microscope (SEM) and optical microscope were used to compute the dimensions of the cantilevers [24]. The stress induced on the wafers was computed using a stylus based profilometer [24]. Figure 7 illustrates the SEM picture of a released cantilevers illustrated in Table 1.

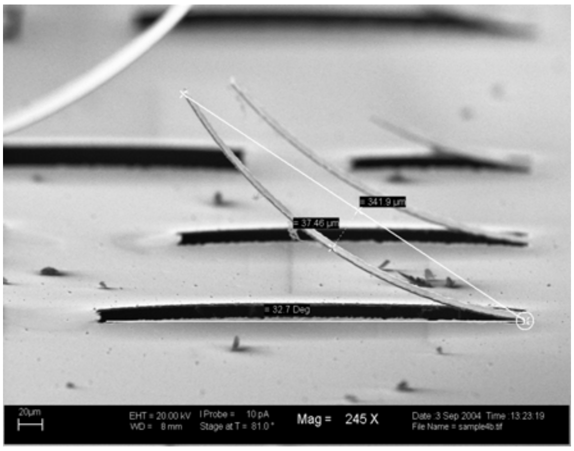


Figure 7: SEM picture of released microcantilevers

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 1: Microcantilevers fabricated at RIT

No.	Stress Al	L_B	W_B	d_B	Thickness Al	Thickness TEOS
Units	MPa	µm	µm	µm	µm	µm
1	27.4	94.24	26.98	53.78	0.41	0.51
2	27.4	100.8	47.62	39.7	0.41	0.51
3	13.67	489.8	61.44	342.5	0.39	0.99
4	13.67	402.8	65.64	255.47	0.39	0.99
5	13.67	205.8	62.64	74.547	0.39	0.99
6	55.49	205.8	64.6	35.10	0.45	2.36
7	55.49	156.6	51.2	11.48	0.45	2.36
8	55.49	485.8	62.3	176.77	0.45	2.36
9	35.92	301.4	41.8	68.119	0.41	2.94
10	35.92	487.4	99.8	112.78	0.41	2.94
11	35.92	207.4	99.8	15.23	0.41	2.94

The above mentioned microcantilevers were modeled in ANSYS with the bulk values for aluminum and TEOS. These simulations were compared to the experimentally obtained data as illustrated in Figure 8. This plot clearly indicates the bulk values are unable to predict the mechanical behavior in the micro domain and alternative techniques are needed to improve the accuracy. On the contrary, the deflections predicted by the effective values are very close to the experimental values. This discussion illustrates the superior performance of the proposed technique.

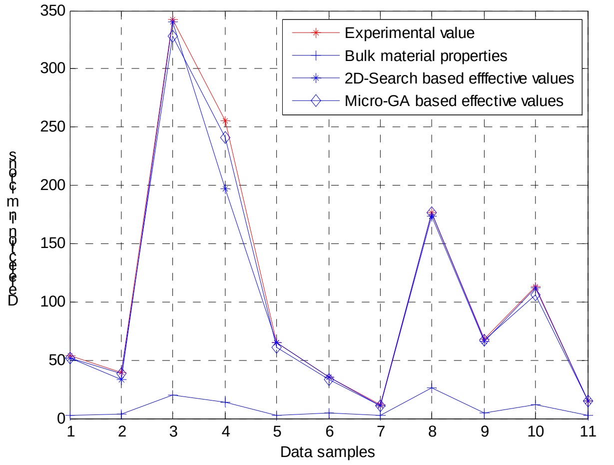


Figure 8: Performance comparison of bulk properties with experimental results

B. Empirical Analysis

The proposed technique estimates the effective Young's Modulus values for aluminum and TEOS using experimental data and finite element analysis. In this process, 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 computed such that the experimental deflections match the simulations. Figures 9 and 10 illustrate the effective Young's Modulus values as computed by 2D search and MGA technique for aluminum and TEOS for the 11 data sets under consideration (Table 1). These figures clearly indicate that the effective values for Young's Modulus are almost an order of magnitude lower than the bulk value. In the case of aluminum, these results are in the same range as reported in literature [11].

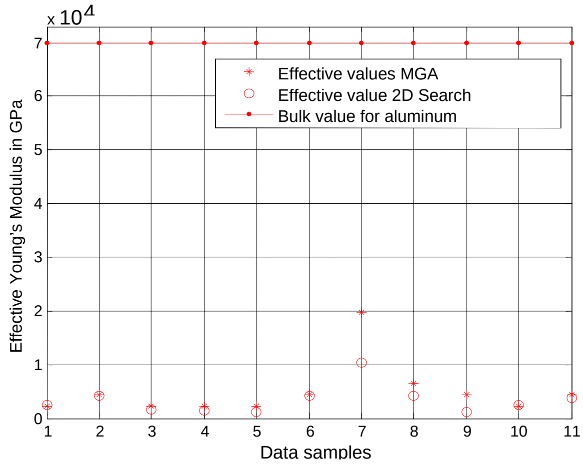


Figure 9: Effective Young's Modulus for aluminum

Also, 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.

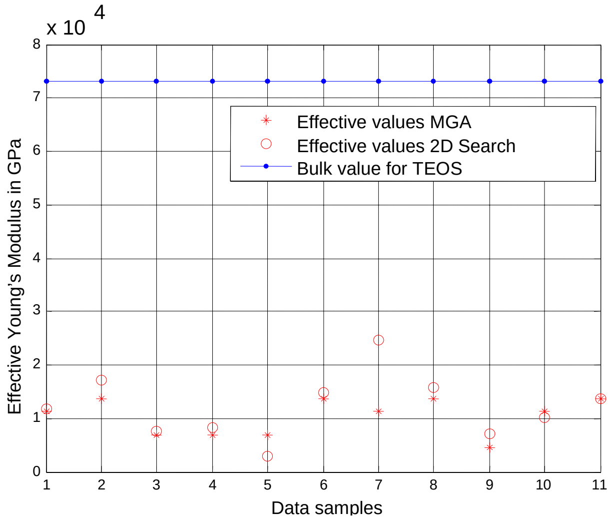


Figure 10: Effective Young's Modulus of TEOS

Figure 11 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.

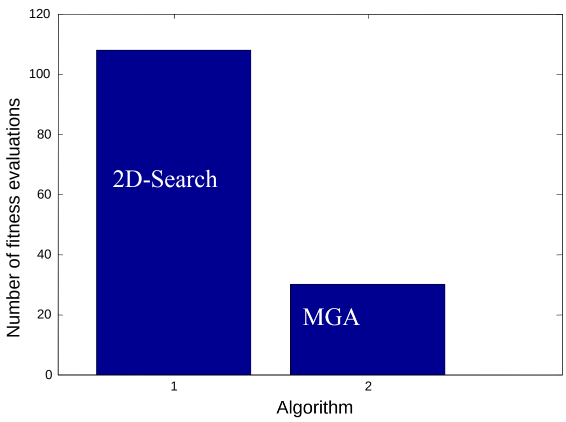
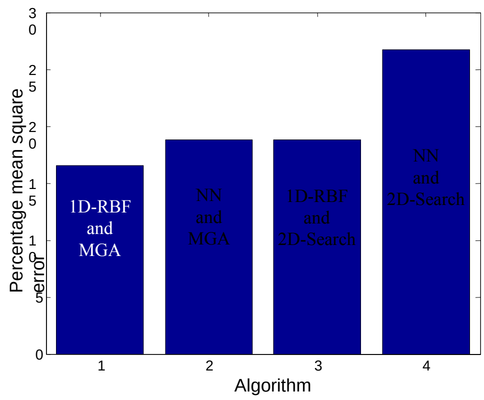


Figure 11: Performance evaluation of the search techniques based on the number of fitness evaluations

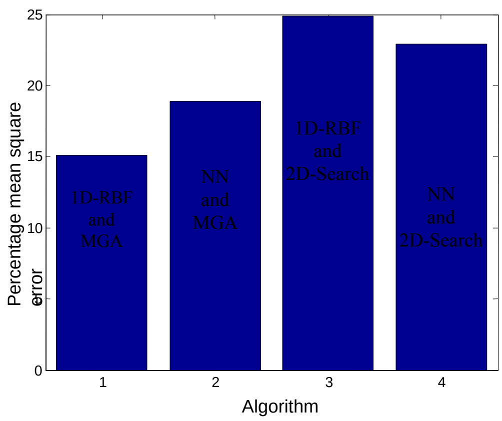
The above generated effective values were then learnt using 1D-RBF networks as well as neural networks. Among the 11 data sets, 7 of them were used for training the networks and the rest were used for testing (data set numbers 2, 5, 8 and 11). Figures 12 (a) and (b) illustrate the percentage mean square error for aluminum and TEOS respectively. 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 maybe advantageous in situations where there limited amount of fabrication data.

IV. Conclusion

This research focuses on developing empirical models that predict the Young's Modulus of thin films of aluminum and TEOS. This was achieved by fabricating micromachined bilayer cantilevers of various dimensions and analyzing the data with the various soft computing techniques. Empirical models were developed with the help of different search and learning algorithms and their performance was compared. This analysis revealed that the performance of the proposed methodology is superior to the existing methods. In addition, the effective values generated using this methodology is 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. Research is in progress in identifying the performance of other algorithms such as support vector machines. In addition to this, work is in progress in investigating other novel test structures that can extract other material properties such as coefficient of thermal expansion.



(a)



(b)

Figure 12: Performance comparison of various learning techniques for predicting the effective Young's Modulus. (a) Aluminum, (b) TEOS

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Ajay Pasupuleti received his Bachelors in Electrical Engineering from Madras University, India in 2000. He received his M.Sc. in Electrical Engineering from Rochester Institute of Technology, Rochester, USA in 2002. He is currently pursuing his PhD in the Microsystems PhD Program at Rochester Institute of Technology. His Thesis involves developing of predictive models that can estimate the Mechanical properties of thin films that are extensively used in MEMS. His current fields of interest involve application of soft computing techniques in MEMS, MEMS CAD and Fabrication of Microscale devices. He is a student member of IEEE.

Ferat Sahin received his B.Sc. in Electronics and Communications Engineering from Istanbul Technical University, Turkey, in 1992. He received his M.Sc. and Ph.D. in Electrical Engineering from Virginia Polytechnic Institute and State University in 1997 and 2000, respectively. His thesis included a Radial Basis Functions Networks solution to a real-time color image classification problem. During his Ph.D., he performed research in biological decision-theoretic intelligent agent design and its application on mobile robots in the context of distributed multi-agent systems. In September 2000, he joined Rochester Institute of Technology, where he works as an associate Professor. His current fields of interests are mobile robots, autonomous robots, modular micro robots, MEMS-based microrobots, swarm intelligence, intelligent control, nonlinear control, multi-agent systems, decision theory, distributed computing, and artificial immune systems. He is a member of the IEEE Systems, Man, and Cybernetics Society, Robotics and Automation Society, Computer Society, and the American Association for Engineering Education (ASEE). He has served as the student activities chair for IEEE SMC society between 2001 and 2003. He is currently the Secretary of the IEEE Systems, Man, and Cybernetics Society. He also volunteers in local IEEE activities. He served as the vice-chair of the IEEE Rochester section between 2003 and 2005.