SIMPLIFYING THE DESIGN PROCESS OF A MEMS-BASED NANOSCALE MATERIAL TESTING DEVICE

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ABSTRACT

Micro Electro Mechanical Systems (MEMS) are increasingly used to investigate the mechanical properties of nanoscale structures; however, their design, analysis, and layout are often difficult processes. We present the details of an online tool that simplifies these processes for particular nanomechanical testers. Our test case is based on a MEMS nanoscale material testing system previously created and tested by Espinosa and Zhu. Our tool allows users to easily explore a parameterized design space, simulate resulting performances, and export the designs as parameterized layout arrays in GDS-II format for direct manufacture. The performance attributes of the resulting sensor depend on the properties of the nanoscale sample under examination. We therefore integrate our parameterized lumped model of a carbon nanotube (CNT) together with the MEMS for a more complete representation of a micro/nanosystem. Our results show that our model agrees well with previously reported results and show that such a M/NEMS can be explored and laid-out by novices in minutes. Our tool is accessed online at nanoHub.org.

Keywords: MEMS, Carbon nanotubes, Nanoscale metrology, Sugar, SugarCube

1. INTRODUCTION

MEMS have the potential to provide accurate mechanical characterization of nanostructures such as CNTs and nanowires. The performance of MEMS highly depends on their structural design, which determines the device's sensitivity and ranges of applied or sensed forces and displacements. The design and performance optimization of MEMS often require several weeks of specialized training in the use of computer aided design and engineering tools.

In particular, a MEMS nanomaterial testing device has been developed by Espinosa et al. [1-3], see Figure 1. The chosen stiffness of the actuator and the load sensor are a strong function of the properties of the specimen to be investigated. Such properties need to be tailored for the prescribed nanostructure specimen in order to obtain sufficient or optimal performance [3]. Hence, each nanoscale specimen may require the material testing device to have a completely different set of geometrical and material properties. Optimization using distributed analysis is computationally expensive, time-consuming, and difficult to geometrically parameterize [4]. And analytical models of this device are not readily available.

We therefore develop a parameterized computer model of this MEMS nanomaterial testing device. What is interesting about our approach is that we integrate a carbon nanotube (CNT) model with the microscale device for multi-scale simulation. Such modeling integration allows the user to explore the performance of a proven MEMS tester applied to various nanoscale structures. We modeled both the MEMS and CNT using Sugar; and we export the design to SugarCube. Sugar is a nodal analysis package for 3D MEMS simulation [5], and SugarCube is a novice-friendly online tool for manipulating parameter values of ready-made MEMS that are initially configured using Sugar [6].

Our model allows the user to explore the thermo-mechanical properties of the MEMS device and optimize its response by adjusting geometry, material properties, and variations of CNT properties. Our CNT model provides a structural mechanics based lumped model of Single-walled nanotubes [7] that can be used to simulate a test specimen of the desired chirality, diameter, and length. Our model is expected to benefit those that do not have design expertise with traditional CAE tools, do not have ready access to such tools, or do not have the time or desire to develop a new computer model from scratch.

The rest of the paper is organized as follows: In section 2, we give details of the simulation model of the nanoscale material testing device made in Sugar and SugarCube. In section 3, we give details of the CNT models available in Sugar. In section 4, we discuss the analytical model of the load sensor and the thermo-mechanical actuator. Finally in section 5, we verify our model with the results in [1-3].

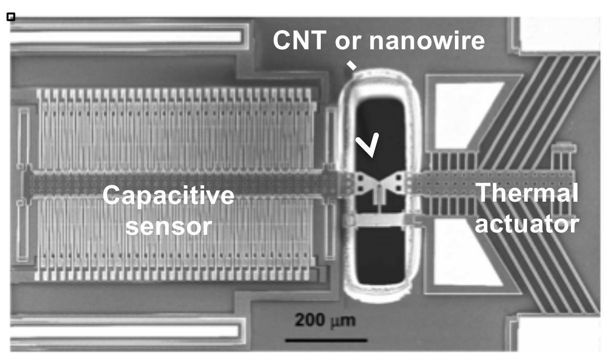

Figure 1: MEMS nanomaterial testing system consisting of a thermal actuator, a capacitive sensor, and a test specimen. By [1-3].

2. MODELING

2.1 Sugar Model

We modeled the MEMS-based material testing device in Sugar [5] (see Figure 2). The design parameters were taken from [1-3]. We parameterized the geometry and material properties of both the device and the CNT test specimen to be used. The device was designed using anchors and electro-thermo-mechanical flexures. The test specimen was modeled using the carbon nanotube models [8]. Static, modal, and transient analyses can be performed on the device with applied force, voltage, or thermal loads. Once a device is configured in low-level Sugar, its netlist can be imported into the novice-friendly high-level SugarCube for easier exploration of design space performance, as well as easy creation of parameterized layout arrays for fabrication.

2.2 SugarCube Model

SugarCube provides novices with simple high-level manipulation controls for ready-made M/NEMS using sliders that are limited by design-rules. Our model is imported into SugarCube after we configured its basic geometry in Sugar using its electro-mechanical netlist language, [5-6]. A multitude of parameters may be chosen to be accessible through SugarCube. In the present example, we choose to demonstrate several parameters for the thermal actuator (V-beam). As seen in Figure 3, sliders appear for V-beam length, width, number, angle, and temperature. We also included parameters for the number of heat sinks and number of comb drive sensor fingers. Static, modal, and transient analyses are available in SugarCube. Upon simulation, parameterized performance 1D values, 2D curves, or 3D manifolds are displayed in the lower-left window (see Figure 3).

Another interesting aspect of SugarCube is that it can generate a parameterized layout array of device in GDS-II format for manufacture [9]. For example, Figure 4 shows an array of the nanomaterial testers, where the rows and columns are parameterized by number and angle of the V-beams. The bonding pad layers and common ground tracers are automatically created for the layout. The layout image in Figure 4 is from using the free GDS-II viewer called CleWin [10]. SugarCube's easy layout generation can reduce the time conventionally spent on layout from days or hours to seconds, and hence can provide significant time and cost savings. For instance, after choosing the two parameters to vary and pressing the *Layout* button, it takes SugarCube 5 seconds to generate the GDS-II parameterized layout shown in Figure 4. MEMSCAP MUMPs design rules are applied.

3. CARBON NANOTUBE MODEL IN SUGAR

We have developed a computer algorithm to model CNTs. Our lumped model is based on the elemental structural mechanics model developed by H. Wan and F. Delale [8]. We imported the parameters of their model into a Sugar electro-mechanical model [5]. Our linear CNT model is parameterized by its radius and length. We use matrix condensation to create a lumped model, see Figure 5. Matrix condensation is use to reduce the number of degrees of freedom of the model without affecting its accuracy. Please refer to [7] for details on our CNT model. In the present work, we integrate our CNT model to emulate more complete nano-mechanical testing conditions to help users choose more appropriate design parameters for the MEMS tester.

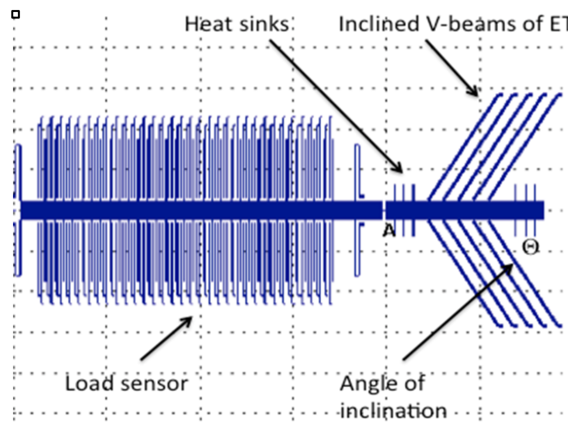

Figure 2: Nanomaterial testing device modeled in Sugar (open source code written in Matlab). The user can efficiently explore the design and performance space with easy to use subnets.

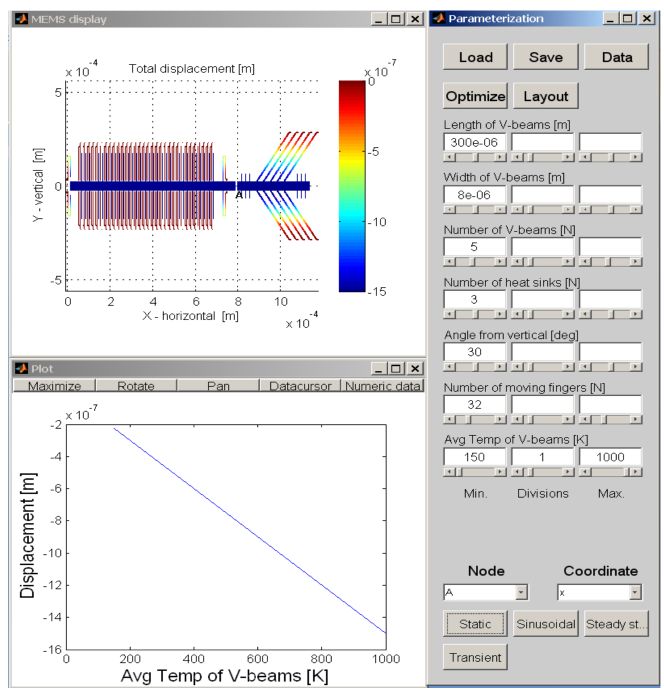

Figure 3: Nanomaterial testing device in SugarCube. In SugarCube, novices can easily modify geometric, material, and CNT specimen parameters using simple sliders. Static, modal, and transient analyses are available. In this instance, the plot shows displacement of the actuator-specimen junction with increase in the average temperature of the V-beams.

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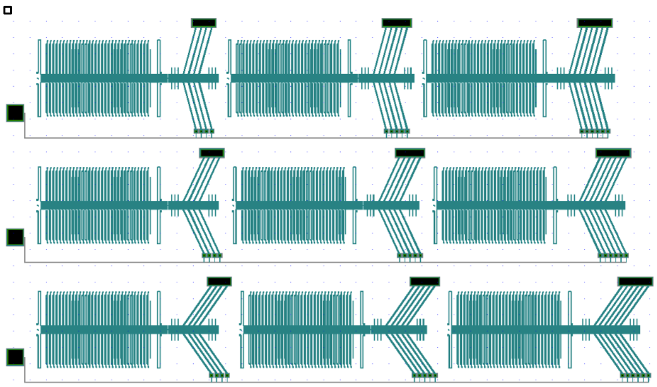

Figure 4: GDS-II layout of an array of nanomaterial testing devices, viewed in Clewin 3.2. The angle and number of V-beams vary along the rows and columns respectively. SugarCube automatically adds tracers and wire bonding pads.

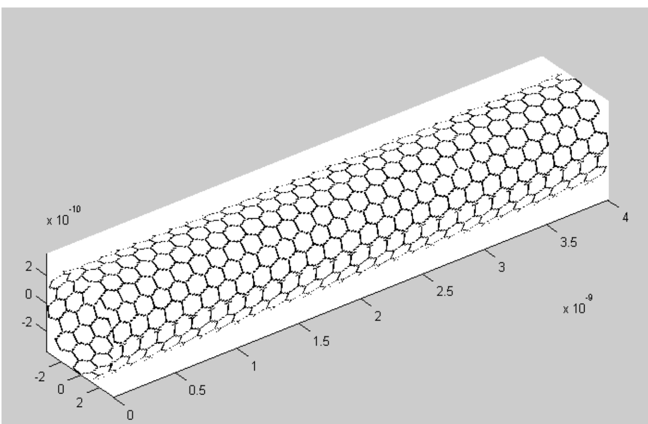

Figure 5: A (10,10) armchair CNT, modeled in Sugar [7]. The model allows the user to simulate symmetrical CNTs (armchair and zigzag) of desired chirality, length, and radius parameters**.**

4. THERMO-MECHANICAL RESPONSE

The nanomaterial testing device consists of an electro-thermal actuator, a test specimen, and a load sensor in series. The governing equations for the lumped model for mechanical analysis of the device are given below [3] (see Figure 6).

$$F_{TA} = F_S = F_{LS}$$

$F_S = K_S \Delta U_S$ and $F_{LS} = K_{LS} \Delta U_{LS}$.

The stiffness of the thermal actuator is given by

$K_{TA} = mK_{tb} + nK_{sb}$, where

$K_{tb} = m\left((\sin\theta)^2 \frac{Ebh}{l} + (\cos\theta)^2 \frac{Eb^3h}{l^3}\right)$ and

$K_{sb} = \frac{2nEb_{sb}^3 h}{l_{sb}^3}$.

The stiffness of the specimen and the load sensor is given by $K_S = \frac{E_S A}{l_s}$ and $K_{LS} = \frac{2Eb_L^3 h_L}{l_L^3}$ respectively.

Finally, the elongation of the specimen is given by

$$\Delta U_S = \frac{2mEA\alpha\Delta T \sin\theta}{\left(K_{TA} + {}^{K_{TA}K_S}/_{K_{LS}} + K_S\right)} .$$

Here *l, b,* and *h* refer to the dimensions of the V-beam; l_{sb}, b_{sb}, and h_{sb} refer to the heat-sink beams; and l_L, b_L, and h_L refer to the folded beams. Also, α is the coefficient of thermal expansion, θ is the beam angle defined from vertical, and E is the Young's modulus of the material used to model the device.

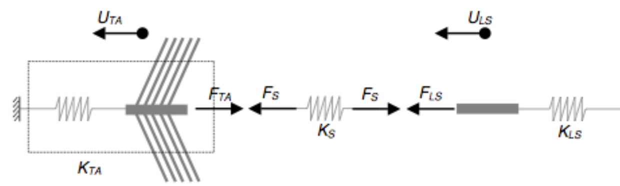

Figure 6: Free-body diagram of the thermal actuator showing internal forces and displacements, from [3].

5. RESULTS

The Sugar model for the MEMS-based material testing device was verified with the results presented in [1-3]. The displacement of the electro-thermo actuator was compared with the finite element analysis (FEA) model given in [1]. An average temperature rise of 55°C was applied to the inclined beam elements. The maximum shuttle displacement was obtained to be 67.5 nm, which corresponded well with displacement given by the FEA model (see Figure 7).

Next, we verified the results of the elongation test with the test data. We modeled a rectangular poly-silicon specimen of length=4.7µm, height=1.6µm and width of 0.42µm. The displacement of actuator specimen junction was found to be 67.5nm for a temperature increase of 55°C for the inclined beam elements. For a temperature increase of 180°C from ambient, this displacement of the actuator-specimen interface was found to be 270.1nm.

For optimum performance of the device, specimen stiffness needs to comparable to that of the load sensor [1]. Hence, for testing the poly-silicon specimen, the width of the folded beams was increased to 35µm. A temperature increase of 350°C was applied to the inclined beams. Using the *cho_dq_view* routine in Sugar, the displacement of the actuator-specimen junction was found to be 387.02nm and elongation of the specimen was found to be 37.93nm. From the analytical model given in Section 4, the specimen elongation was found to be 94.58nm.

We now present the results of integration of the CNT model with the nanomaterial tester. The CNT test specimen of diameter 0.78nm and length 5nm was modeled using the

CNT model [7]. A specimen elongation of 172.8nm was obtained from the Sugar CNT model, for an average temperature rise of 150deg of the inclined beams. For the same specimen, the elongation was found to be 149.6nm from the analytical model.

The discrepancy in the results can be attributed to the following reasons: the geometry of the folded beams highly affects the stiffness of the load sensor and in-turn the calculated specimen elongation. We have modeled the folded beams as rectangular beam elements, instead of arch-shaped structures. Also currently, a distributed temperature profile is not applied to the lumped elements in Sugar. Hence, the complete length of the V-beam is maintained at a high constant temperature; and the heat sinks and shuttle is maintained at room temperature. To be more accurate, proper effects of temperature gradients need to be addressed.

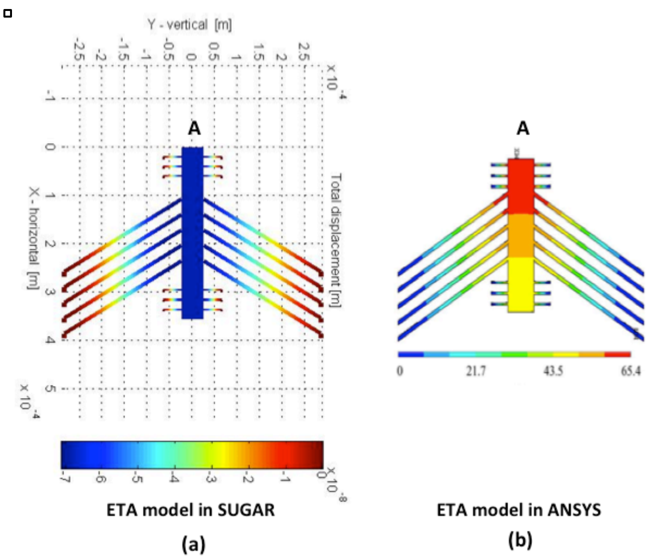

Figure 7: Displacement a thermal actuator subject to a temperature increase 55 °C in the V-beams. Here, y-direction displacement of point 'A' is shown in nanometers for (a) our lumped model in Sugar, (b) Espinosa's distributed model [1]. Note: displacement map colors between Sugar (left) and ANSYS (right) are reversed.

6. CONCLUSIONS

In this paper we introduced a novice-usable online tool to simplify the designing of the MEMS-based nanoscale material testing device. We also discussed the integration of carbon nanotubes with the mechanical and thermal properties of the micro-scale device. Our model allows the user to optimize the performance of the device by adjusting geometry, material properties, and variations of CNT test specimens. Our SugarCube based model can generate layout of an array of the device in GDS-II format for direct manufacture. This simulation tool will highly benefit both experts and novice users. Our effort significantly reduces design optimization time and overall manufacturing time for the device.

Currently, we are creating a voltage-driven electro-thermal model for Sugar. Such a model will allow users to integrate control electronics. And future developments of models that more completely simulate the thermodynamics involved are expected to increase the accuracy of this nanomaterial testing device in SugarCube.

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REFERENCES

[1] H.D. Espinosa, Y.Zhu, N. Moldovan, "Design and Operation of a MEMS-Based Material Testing System for Nanomechanical Characterization", *Journal of Microelectromechanical Systems*, Vol. 16, No. 5, pp. 1219-1231, 2007.

[2] Y. Zhu, H.D. Espinosa, "An electromechanical material testing system for in situ electron microscopy and applications", *PNAS*, Vol. 102, No. 41, pp. 14503-14508.

[3] Y. Zhu, A. Corigliano, H.D. Espinosa, "A thermal actuator for nanoscale *in situ* microscopy testing: design and characterization", *Journal of Micromechanics and Microengineering*, Vol. 16, No. 2, pp. 242-253, 2006.

[4] Z. Bai, D. Bindel, J. Clark, J. Demmel, K.S. J. Pinter, N. Zhou, "New numerical techniques and tools in SUGAR for 3D MEMS simulation", *in: Technical Proceedings of the Fourth International Conference on Modeling and Simulation of Microsystems*, pp. 31–34, 2000.

[5] J. V. Clark, K. S. J. Pister "Modeling, Simulation, and Verification of an Advanced Microdevice Using Sugar," Journal of Microelectromechanical Systems, Vol 16, No 6, Dec 2007.

[6] P. Marapalli, J. V. Clark, "An Online Tool for Investigating the Performance of Ready-Made Parameterized MEMS", *Nanotech 2010, International Conference on Modeling and Simulation of* Microsystems Anaheim CA, June 21-25, 2010.

[7] R. Bansal, J.V. Clark, "Simplifying the Designing of a MEMS-Based Nanoscale Material Testing Device", *in Proc. NanoTech 2011,* Boston, 2011.

[8] H. Wan, F. Delale, "A structural mechanics approach for predicting the mechanical properties of carbon nanotubes", *Meccanica*, Vol. 45, pp. 43–51, 2010.

[9] P. Marepalli, J.V. Clark, "An Online MEMS Design Tool that Lays Out and Simulates a Parameterized Array from a Reference Device", *in Proc. NanoTech 2011*, Boston, 2011.

[10] CleWin - WieWeb Software, Achterhoekse, Molenweg 76, 7556 GN Hengelo, The Netherlands http://www.wieweb.com/nojava/layoutframe.html