

# **An Application of Stochastic Methods to Develop Hybrid Finite Element Models of Nanostructures**

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## **SUMMARY**

**In the early 1960s when finite element methods were in their infancy, rocket scientists used bars and shear panels with fictitious properties to successfully model solid propellant grains. In that same era Monte Carlo computer simulations were used to design real time flight load measurement systems. These early computer simulations, which involved the author, were motivation for this paper that applies stochastic methods to create fictitious properties data for finite element models of nanostructures. A hybrid shell-beam finite element model of a (9,0) zigzag carbon nanotube was created using stochastic methods to find fictitious beam section properties. The resulting hybrid model produced excellent equivalent-continuum results and an all beam model produced vibration modes for a nanomechanical resonator in general agreement with published results.**

## **1 INTRODUCTION**

**Over the last fifty years finite element models have been used to simulate engineering structures ranging from huge vehicle assemblies to tiny MEMS devices. In virtually all these applications the objects modeled are above the molecular scale. At the nanoscale elastic properties of carbon nanotubes have been studied extensively [1,2]. Recent work at NASA [3,4] systematically developed equivalent-continuum models for nano-structured composite materials. In that work**

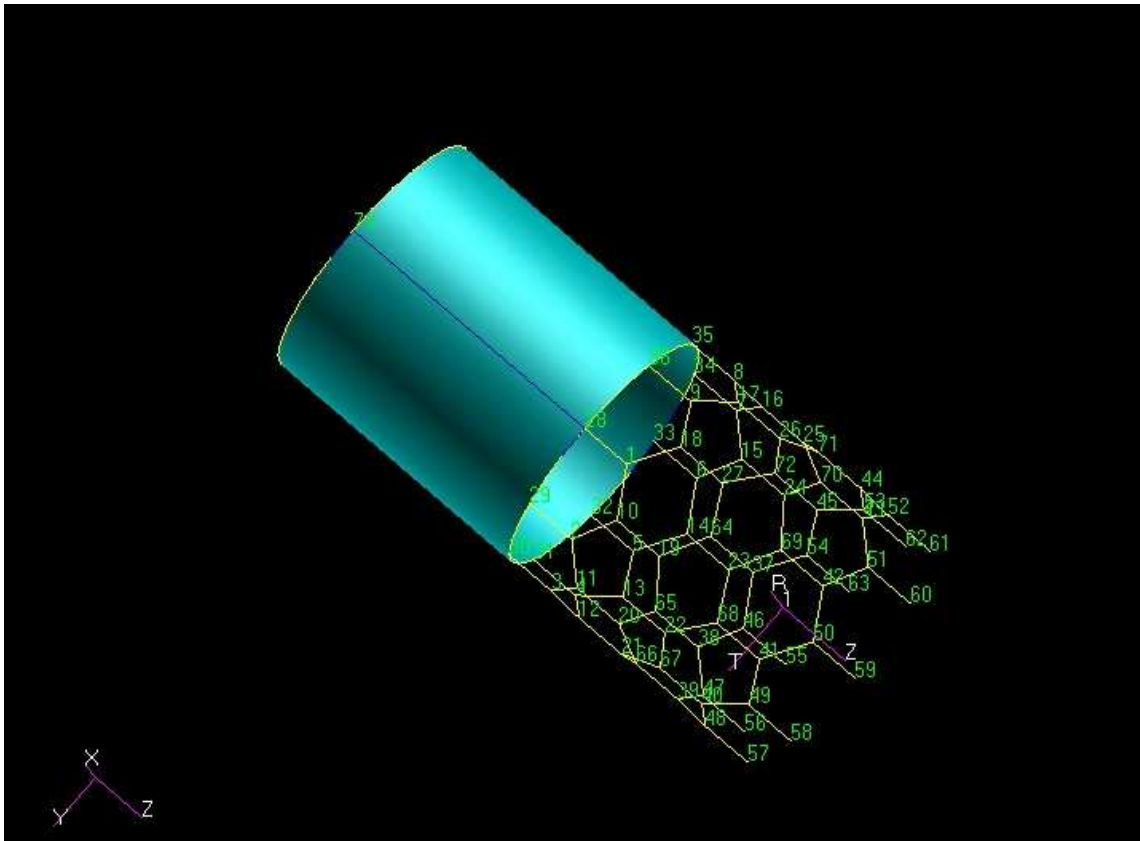
both molecular and equivalent-continuum finite element simulations were used. The scope of the present paper is limited to equivalent-continuum mechanics models for carbon nanotubes. This study uses finite element models different from NASA's. Our choice of beam elements rather than truss and panel elements is similar to that of Chou [5] and many others. A stochastic methodology is used to create fictitious finite element property data. Beam element section properties were determined using Monte Carlo simulations to search for fictitious section property values that would produce equivalent-continuum deformations in a hybrid shell-beam nanotube model. The hybrid model and a nanomechanical vibration model using only beam elements were computationally tested under a variety of loading conditions.

In an earlier heuristic finite element study [6] Armchair (n,n) carbon nanotubes were modeled using beam elements. In this study a (9,0) Zigzag nanotube is modeled using shell elements for one-half of the nanotube and beam elements for the other half. Stochastic design Improvement software was used to help find beam section properties that produced equal work in deforming each half of the model. We demonstrated that a hybrid FEM assembly of continuum shell and discrete beam elements could simulate the elastic deformations of a carbon nanotube for static and dynamic loads. Evaluation testing included stretching, bending, and vibration deformation modes. Next a nanomechanical resonator was modeled using only beam elements and virtual vibration tests run for the first 10 modes. The paper concludes with a discussion of ways this methodology might be used to embed skeletal finite element models in a soft matrix solid like a

human cell. Molecular level models embedded directly in equivalent-continuum models of solids are possible with modern meshing tools. Even today the mechanics of cells are modeled using finite element spring models in textbooks [7].

## 2. NANOSCALE FINITE ELEMENT MODELS

Avagadro's number is usually defined as the number of carbon atoms (  $6.22142 \text{ E}+23$  ) in 12 grams of carbon-12. In general it is the number of "molecules" in one mole of a substance. Point elements (atoms) in the beam finite element half of the nanotube model, Figure 1, have a mass determined with Avagadro's number. This is the bridge between atomic and continuum mass models. In this paper all the properties are in nanometers so for example Young's modulus is in  $\text{N}/\text{nm}^{**2}$  and not in Pascal's which are  $\text{N}/\text{m}^{**2}$ . That shifts the modulus exponent by 18 and some computer analyses can produce "overflow" errors if inconsistently scaled units are used. Other than attention to detail with unfamiliar nanoscale units and introductory quantum mechanics the FEM model was not difficult to build or analyze.



**Figure 1. Hybrid Shell-Beam Finite Element Model**

Atomic coordinates for the zigzag (9,0) nanotube were computed using Saito's code [1] for a unit cell and imported into MSC Patran as a neutral file. The shell element thickness used for continuum models of a SWNT is based on the interlayer thickness,  $t = 0.34$  nm, of graphene in graphite crystals. The recent NASA work used  $t = 0.28$  nm for their truss and panel equivalent-continuum models. That value would create a mass imbalance in the present hybrid models for vibration analyses if graphite's mass density was used for the shell elements. Fictitious beam section properties for equivalent-continuum static analyses were found for both shell thicknesses but only the graphene sheet thickness was used for vibration analyses. The shell elements mass density was graphite's  $2.2E-31$  g/nm<sup>3</sup>.

## Monte Carlo Methodology

Current use of Monte Carlo (stochastic) simulation in design and analysis is well documented, [8,9]. Earlier use of Monte Carlo simulations to design real time flight load measurement systems is documented only in lab papers of that era, Meriwether [10]. He monitored dozens of randomly applied strain gages on a complex structure during a series of uniaxial stretching and uniaxial bending calibration tests. The calibration data were then used to randomly create thousands of virtual Wheatstone bridges using an ancient IBM 650 computer. The probability of finding a Wheatstone bridge circuit that responded only to a pure axial or a pure bending flight load was surprisingly high because the number of possible circuits with N gages is:  $N(N-1)(N-2)(N-3)/8$ . Aircraft carrier landing tests later proved the flight loads instrumentation based on this methodology was very accurate [10]. Subsequently in a 1961 interceptor missile flight test we used the same methodology to successfully measure canard control fin dynamic loads during hypersonic maneuvers.

Meriwether's work inspired the methodology used in this paper. Sequential Monte Carlo design scans are used to find fictitious section properties for the beam elements in a hybrid FEM model of a carbon nanotube. The specific tool was Stochastic Design Improvement (SDI) in MSC Robust Design, Figure 2. It searches each Monte Carlo scan to find a design with properties that best meet preset goals. The goal specified for static simulations was equal work hence equal axial deformations in each half of the hybrid model. Beam element area and moments of inertia were allowed to

vary randomly during each Monte Carlo search. The shell element thickness was kept constant.

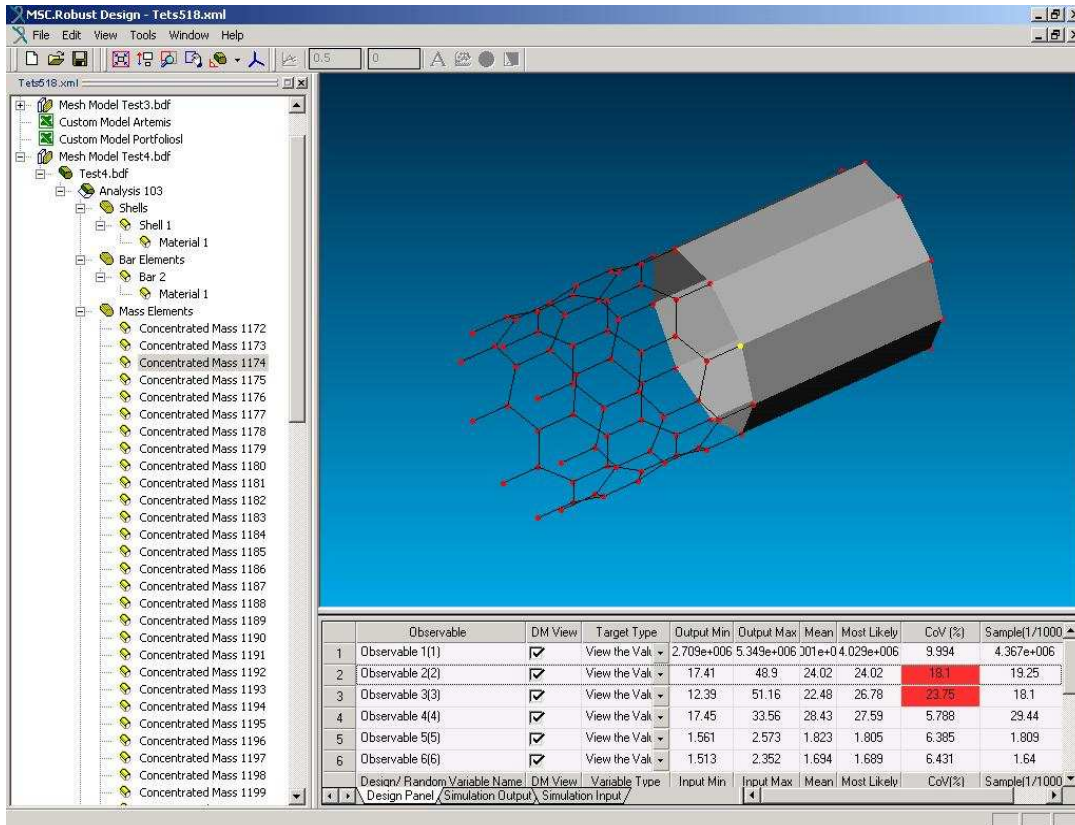
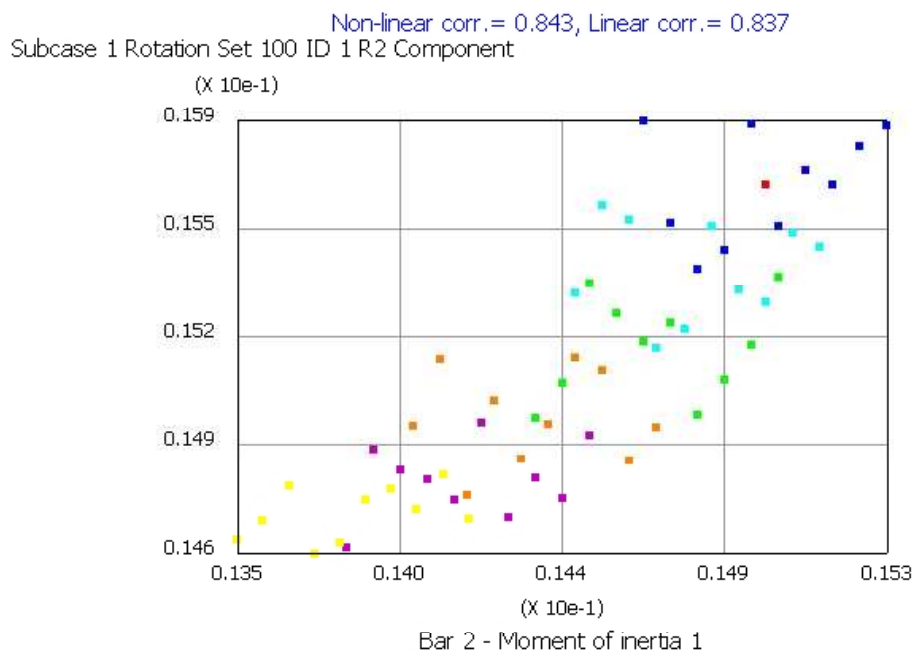
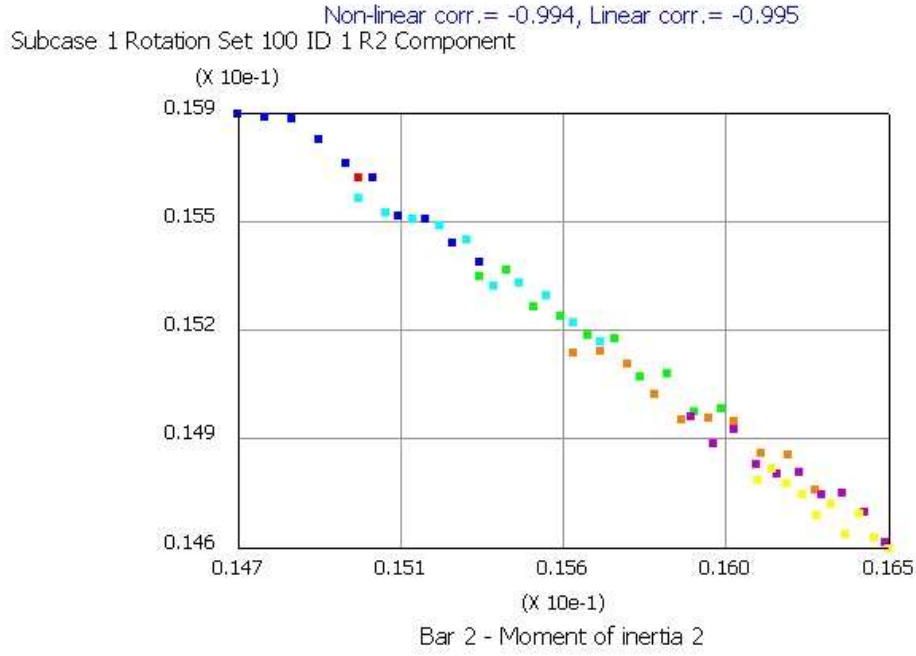


Figure 2. Stochastic FEM Property Simulation Model

The carbon-carbon bonds in a nanotube stretch, bend and twist when loaded [11]. Chou [5] describes how a beam's fictitious elastic properties, EA, EI, and GJ can be related to three molecular mechanics force field constants [12]. In this paper the beam fictitious properties were found using a hybrid beam-shell model with shell elastic properties taken from the SWNT literature [2a]. In other words the energy balance calculation was made at the equivalent-continuum level for nanotube mechanics. SDI results from the FEM model showed, as expected, that the fictitious beam cross-sectional area dominates nanotube elastic

response. After finding the area that produced equal axial deformations, beam moments of inertia were used to fine tune the slope at mid-length to near zero for symmetric bending deformations.

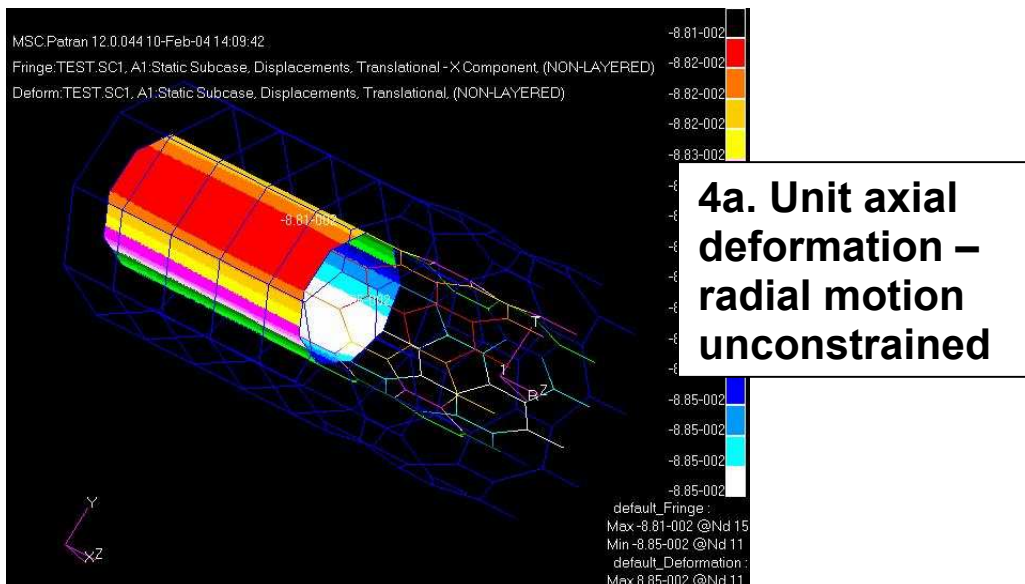
There are two bending moments of inertia and a torsion moment of inertia available in a standard beam element property model. In the heuristic spirit of this paper we tested all three in the SDI Monte Carlo scans. Interestingly the two bending moments of inertia have opposite effects on the slope at mid-length, Figure 3. The torsion constant had little if any effect on nanotube mid-length slope. The SDI runs were very helpful in getting an approximate solution and final calibration work was done interactively.

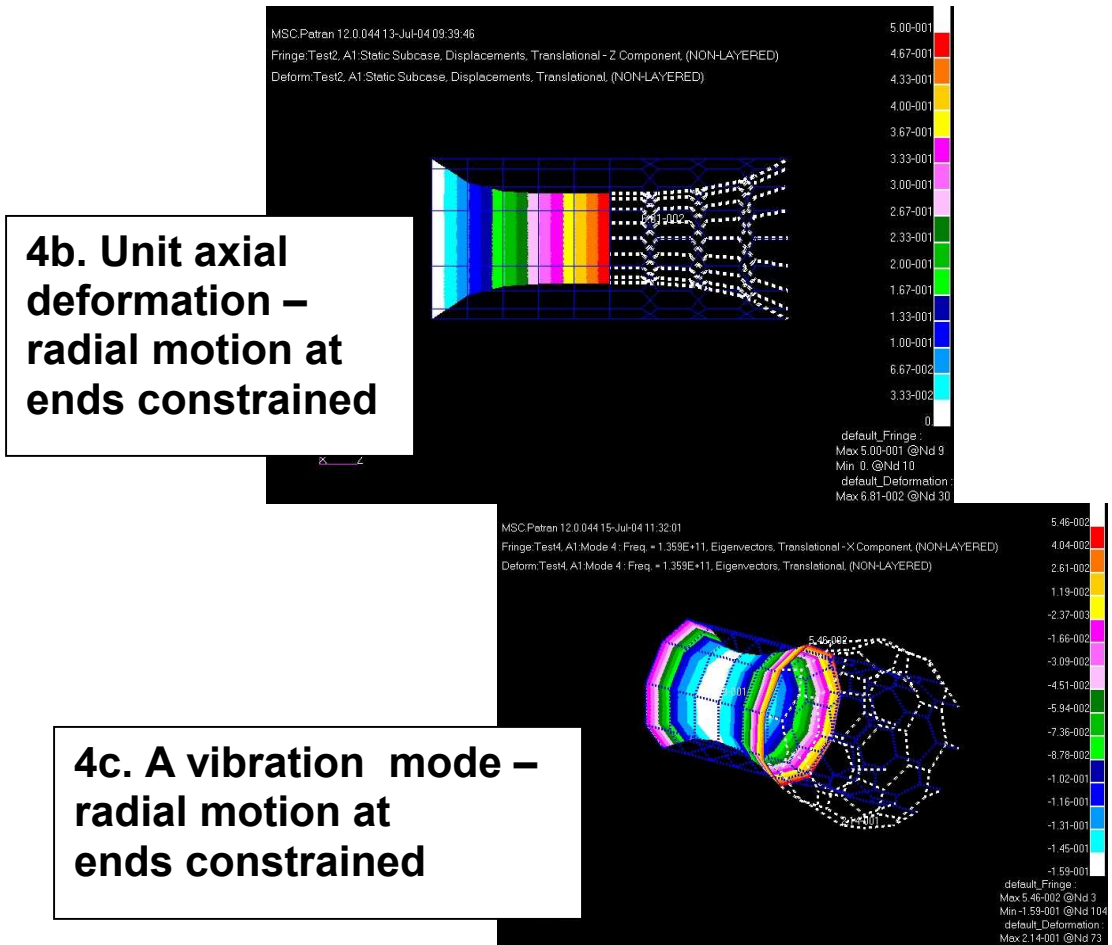


**Figure 3. Mid-length slope for random  $I_1$  and  $I_2$  values**

### 3. NANOSCALE FINITE ELEMENT ANALYSES

After work-equivalent beam section properties were found, a series of computational experiments were run. The first hybrid model was the (9,0) zigzag nanotube, Figure 2, with  $L = 1.562$  nm. The first test case, Figure 4a, was a unit axial stretching of the tube unrestrained in the radial direction. This model also had been used in the SDI scan to find the beam cross-section area that produced an axial deformation of  $\frac{1}{2}$  at mid-length. The axial test produced a constant radial deformation full length with less than 1.0% variance.





**Figures 4 Hybrid Finite Element Elastic Deformations**

End boundary conditions then were fixed to introduce a symmetric bending deformation. Testing included compression as well as tension. Note that in Figures 4a,b,c only the radial component of deformation is imaged in order to magnify the behavior of the hybrid model at mid-length. The unit stretch load cases have large axial displacement components and showing only the resultant deformations would mask the small bending response caused by the end radial constraints.

The last hybrid model test was for a vibration analysis. The results were encouraging, Figure 4c. A G-band mode shape, Figure 5, was found much like those seen

in Raman spectra for a SWNT. The hybrid model length and boundary conditions were different from the unit cell vibration models analyzed in the literature [13,14]. Raman spectroscopy uses light in the infrared frequency range to excite SWNT vibrations. Experimental results are reported in  $\text{cm}^{-1}$  wavelength units that require another unfamiliar units conversion. To obtain the Raman frequency in Hz units compute  $f = 2\pi c \omega$  where  $c$  is the speed of light in cm/s and  $\omega$  is the Raman wave number.

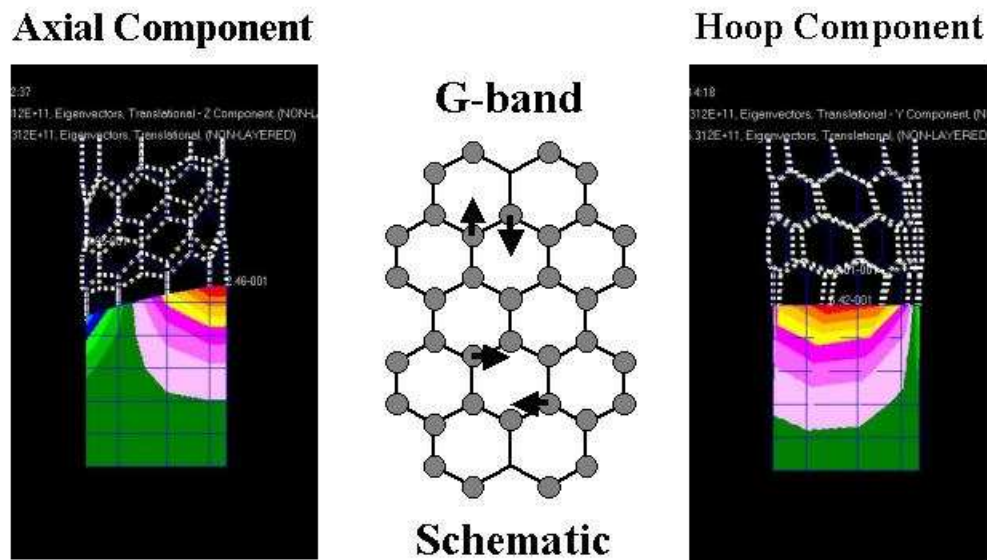


Figure 5. Schematic of G-band mode atomic vibrations

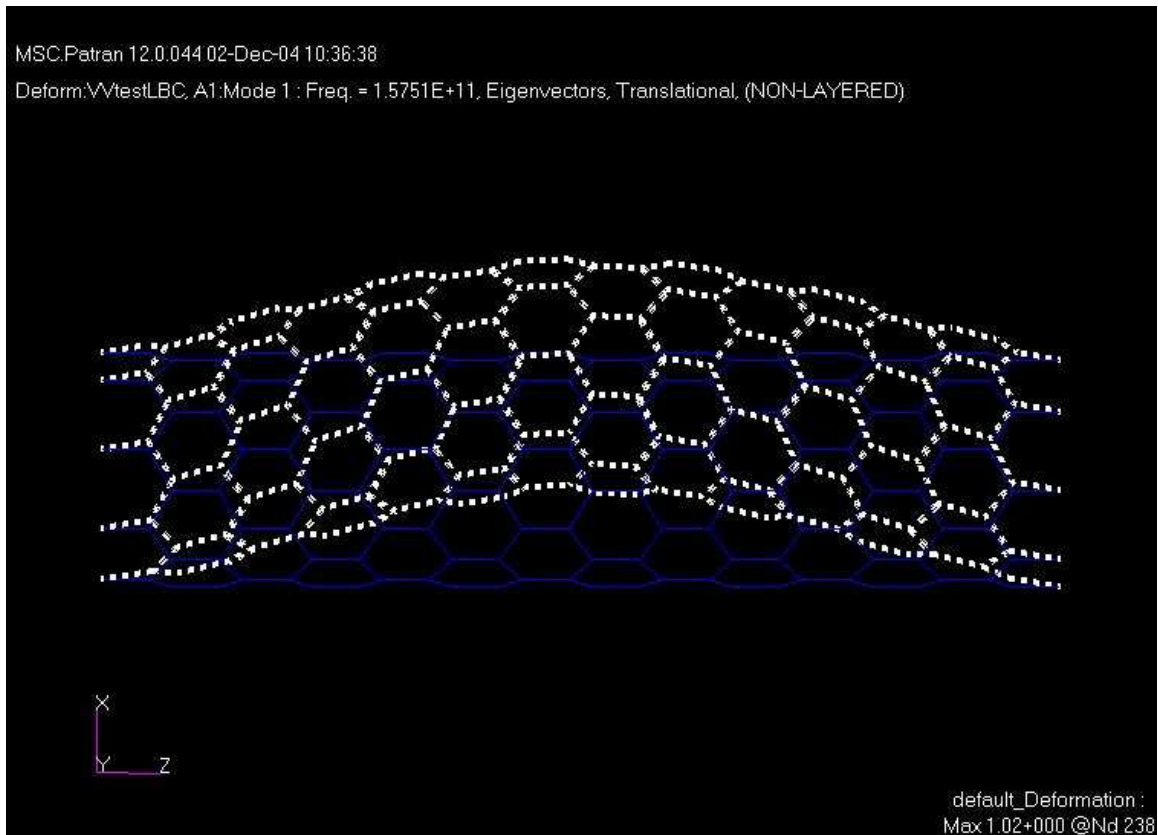
The hybrid model G-band eigenvector components for axial and hoop deformation are shown in Figure 5. They are basically in-plane only motion, but the frequency was lower than expected. The Raman G-band frequency for a SWNT is about  $1500 \text{ cm}^{-1}$  and that will require

further study of the hybrid model to reconcile boundary condition effects at a minimum.

## Nanomechanical Resonator

Industrial interest in nanomechanical resonators is high because of their extremely high vibration frequencies, 10GHz to 1.5THz, depending on the nanotube diameter and length. One application is as a sensor for mass detection at the atomic level. They could, for example, detect minute traces of a gas or a virus [5]. An actual nanomechanical resonator was lab tested recently by Mc Euen and others [16] using electromechanical excitation. This was in a circuit and the tube was quite long reducing the vibration mode frequencies to less than 200 MHz. Even at these lower frequencies there are many potential applications in the radio-frequency range.

An all beam element model, Figure 6, was constructed similar to [5] and the first 10 vibration modes were computed. This test was to compare the nanomechanical property model with the beam model based directly on force field constants for EA, EI and GJ. The first mode for bridged boundary conditions had a frequency of  $1.5 \cdot 10^{11}$  Hz. This is in the frequency range reported in [5] with no attached mass,  $10^{11}$  to  $10^{12}$  Hz, for different length tubes. However, the tube analyzed here was shorter,  $L = 2.911$  nm, than those analyzed in [5] so that the  $1.5 \cdot 10^{11}$  Hz frequency is lower than expected. Additional modeling work is planned to create longer tubes in the same range as those analyzed in [5].



**Figure 6. Nanomechanical resonator FEM model**

#### **4. CONCLUSIONS AND RECOMMENDATIONS**

The motivation for this research was the same as NASA's and DARPA's nanotechnology research work. New materials and products that nanotechnology is making possible require design tools that bridge the gap between atomic, molecular and continuum mechanics. Many studies have established the utility of finite element models for analyzing nanostructures. In this paper a hybrid model bridge between continuum and nanomechanical FEM models was demonstrated. One potential utility of a hybrid model is its ability to resolve global and local behavior in one simulation. The feasibility of that was demonstrated for a zigzag carbon nanotube.

**The Monte Carlo methodology used here to create fictitious properties for nanomechanical FEM models is not specific to carbon nanotubes. It could be used for any nanostructure model not just hybrid models. The basic requirement is a continuum level property to calibrate against. Regular structures like the carbon nanotube can be modeled easily using universal force field constants [5] but the training required is usually not found in a design group. When more complex nanostructures must be modeled that statement is even truer. Hopefully the methodology described here will help make nanomechanical models more accessible to designers of nanostructures and materials [15].**

**Finally a recommendation for future research in meshing technology for embedded molecular structures in continuum solid models. The general concept is not new as meshing with hard-point constraints is widely available. The extension of this approach to hard-line constraints for molecular covalent bonds embedded in a solid continuum is feasible today. A cytoskeleton embedded in a cell modeled as a continuum solid is an application that would be very interesting.**

## **5. ACKNOWLEDGEMENTS**

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