International Journal of Electrospun Nanofibers and Applications, Vol. 3, No. 2 (July-December, 2017)
ISSN : 0973-628X

Vibration Analysis of Pre-Stressed Single Walled CNT Based Mass Sensor

Ashok Boda, Anand Y. Joshi, Satish C. Sharma & S. P. Harsha

Mechanical & Industrial Engineering Department, Indian Institute of Technology Roorkee Roorkee–247 667, India

Abstract: *Carbon nanotubes (CNTs) are molecular-scale tubes of graphitic carbon with good mechanical, outstanding and unique electrical, thermal, and optical properties. Due to these properties they are suitable for a wide range of applications, such as field emission, nano–sensors and nano–actuators, etc. This article provides determination of natural frequency and various mode shapes of Single walled Carbon nanotubes (SWCNTs) through Finite Element Method (FEM) based software. Additionally, this study explores the resonant frequency shift of the single–walled carbon nanotubes caused by the addition of a nano–scale particle on the beam tip and at various intermediate positions. In order to explore the suitability of the single–walled carbon nanotubes as a mass detector device for many sensing applications, the simulation results for the resonant frequency are compared to the numerical results obtained by the Rayleigh–Ritz method for the beams having no nano–particle and with a nano–particle on the tip or at various intermediate positions along its length. It is shown that the finite element method simulation results are in good agreement with the numerical results, and the discrepancy of the FEM simulated result and Numerical methods have been found approximately less than 10%. Hence the modeling approach is suitable as a coupled–field design tool for the development of single–walled carbon nanotube based mass sensors.*

Keywords: *MASS SENSOR, CNT, SWCNT, FEM*

1. INTRODUCTION

Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are amongst the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. Carbon nanotubes possess exceptionally high stiffness; strength and resilience, as well as superior electrical and thermal properties. CNTs provide the ultimate reinforcing materials for the development of nanotubes. Typically, carbon nanotubes are long tiny cylinders of graphite structure with cap at each end. The length and the outer diameters usually extend from about 2.5nm to 30nm. The most important features of carbon nanotubes are their extremely high stiffness combined with excellent resilience.

CNTs are hexagonal networks of carbon atoms of approximately 1 nm diameter and 1 to 100 microns of length. They can essentially be thought of as a layer of graphite

corresponding author: surajfme@iitr.ernet.in

rolled up into a cylinder [1]. CNTs are of different sizes and forms when they are dispersed in a matrix to make a nanocomposite. They can be single walled or multiwalled with length of a few nanometers or a few micrometers, and can be straight, twisted and curled, or in the form of ropes. Their distribution and orientation in the matrix can be uniform and unidirectional or random in nature. The application of CNTs in next – generation of sensors has the great potential of revolutionizing the sensor industry due to their inherent properties such as small size, high strength, high electrical and thermal conductivity, and high specific surface area [2, 3].

Moreover, nanotubes have been utilized as nano sensors [4], and nano actuator [5]. CNTs have many distinct and unique properties that may be exploited to develop next generation sensors. The main requirements of a good sensor are extreme sensitivity, low cost, low power consumption high reliability and fast response. Several studies have been investigated that CNTs can be used as a mass sensor [5, 8]. The use of vertically aligned SWCNTs for field emission and vacuum microelectronic devices, and as nano-sensors, and nano-actuators, is being actively explored [6,7]. Generally the simulation models for CNTs can essentially categorized as discrete or continuum models. Discrete models that can be treated as Molecular Dynamics (MD) models have been widely applied in nano scale research [9]. In this study, the potential of SWCNT based resonanators have been examined. Resonance based sensors offer the potential of meeting the high performance requirement of many sensing applications, including chemical reaction monitors, metal deposition monitors, biomedical sensors, mass detectors etc. [10 -13]. Also the Carbon nanotubes (CNTs) have been suggested as the basic elements of nanoelectromechanical systems, such as nanobalance [5], nano oscillator [14], and nanotweezers [15]. The principle of mass detection using resonators is based on the fact that the resonant frequency is sensitive to the resonator mass, which includes the self-mass of the resonator and the mass attached on the resonator. The change of the mass attached on the resonator can cause a shift of the resonant frequency.

In this article we have followed the continuum mechanics with the Finite Element Method (FEM) approach to find out the vibration response of individual carbon nanotubes, treated as cylindrical beams or thin shells with thickness. The use of FEM software provides a fast computation of mechanical and vibration responses of carbon nanotubes. In this article the vibration response of SWCNTs and various mode shapes has been analyzed. Furthers this study explores frequency change caused by change in the carbon nanotube dimensions in terms of change in length as well as diameter, and also the addition of mass on the tip of the carbon nanotube and anywhere along the length of the nanotube. The simulation results for the resonant frequency are compared to the numerical results obtained by the Rayleigh–Ritz method for the beams without nano–particle and those with a nano–particle on the tip or at various intermediate positions along its length.

2. PROBLEM FORMULATION

In general, all the systems existing in nature physically belong to the continuous system, where it is not possible to identify discrete masses, dampers, or springs. All the continuous systems are having infinite degrees of freedom. For solving these continuous systems by exact methods and to determine their natural frequencies is a very cumbersome task because the actual solution of these determinants is of higher order which becomes more and more difficult with increasing number of degree of freedom. It may be realized that the vast majority of continuous systems lead to eigenvalue problems that do not lend themselves to closed–form solutions, owing to non-uniform mass or stiffness distributions. Hence quite often it is necessary to seek approximate solutions of the eigenvalue problem. There are several approximation methods available for solving the eigenvalue problems. Here, in this analysis we have used the Rayleigh-Ritz method to get the system's natural frequencies.

Rayleigh's method is a procedure designed to estimate the fundamental frequency of a system without solving the associated eigenvalue problem. The method is based on Rayleigh's principle, which can be stated in the form: "*The estimated frequency of vibration of a conservative system, oscillating about the equilibrium position, has a stationary value in the neighborhood of a natural mode.*"

This stationary value is a minimum in the neighborhood of the fundamental mode.

Rayleigh's method can be applied to find the fundamental natural frequency of continuous systems. The natural or fundamental frequency of the continuous system can be solved by using the Rayleigh's quotient.

$$R(Y) = \lambda = \frac{V_{\max}}{T_{\max}} = \omega_n^2 = \frac{\int_0^l EI\left(\frac{d^2Y(x)}{dx^2}\right)^2 dx}{\int_0^l \rho A (Y(x))^2 dx} \tag{1}$$

Where $V_{\max}$ is the maximum potential energy and $T_{\max}$ is the maximum kinetic energy of the beam

Hence, for any trial function or deflection curve $Y(x)$ resembling the fundamental mode $Y_1(x)$ to a reasonable degree, Eq. 1 yields an estimate for the first eigenvalue ω_1^2 or λ and $R(Y)$ is called the Rayleigh's quotient.

The Rayleigh – Ritz method can be considered as an extension of Rayleigh's method. It is based on the premise that a closer approximation to the exact natural mode can be obtained by superposing a number of assumed functions than by using a single assumed function, as in Rayleigh's method. If the assumed functions are suitably chosen, this method provides not only the approximate value of the fundamental frequency but also the approximate values of the higher natural frequencies and the mode shapes. An arbitrary number of functions can be used, and the number of frequencies that can be obtained is equal to the number of functions used. A large number of functions, although it involves more computational work, lead to more accurate results.

In the case of transverse vibration of beams, if n functions are chosen for approximating the deflection curve $Y(x)$, one can write

$$Y(x) = c_1 y_1(x) + c_2 y_2(x) + \ldots\ldots + c_n y_n(x) \tag{2}$$

Where $y_1(x), y_2(x), \ldots\ldots. y_n(x)$ are known linearly independent functions of the spatial coordinate x, which satisfy all the boundary conditions of the problem and $c_1, c_2, \ldots.. c_n$ are coefficients to be found. The coefficients c_i are to be determined so that the assumed functions $y_i(x)$ provide the best possible approximation to the natural modes. To obtain such approximations, the coefficients c_i are adjusted and the natural frequency is made stationary at the natural modes.

To make the natural frequency stationary, we set each of the partial derivatives equal to zero and obtain

$$\frac{\partial \omega_n^2}{\partial c_1} = 0, \frac{\partial \omega_n^2}{\partial c_2} = 0, \frac{\partial \omega_n^2}{\partial c_n} = 0 \tag{3}$$

Solving the Eq. 3, we get a set of i homogeneous linear equations in unknowns $c_1, c_2, \ldots. c_n$. This defines an algebraic eigenvalue problem similar to the one that arise in multi-degree of freedom systems and also contains the undermined quantity ω_n^2. It will have a non–trivial solution if the determinant of its coefficients is equal to zero. This leads to an i^{th} degree equation in ω_n^2, the solution of this eigenvalue problem generally gives n natural frequencies $\omega_n^2, n = 1, 2, 3\ldots\ldots.n$ and n eigenvectors, each contains a set of numbers for $c_1, c_2, \ldots. c_n$, the lowest root of which is a good approximation to ω_{n1}^2.

The expression for Rayleigh's quotient depends on the system considered. Moreover the trial functions used in the quotient must satisfy all the boundary conditions of the problem. In this article, the system, i.e. CNT is considered as continuous one and the general expression for the continuous system is as follows.

Case 1: Let us consider the eigen value problem associated with a longitudinal vibration of a thin uniform rod of carbon nanotube, clamped at the end $x = 0$ and free at the end $x = L$. Consider carbon nanotube as a uniform beam of length l and ρ is the density of the material and A is the cross sectional area of the CNT beam, E, I are the young's modulus and moment of inertia of the CNT respectively. And m is the mass of the CNT considered, EA(x) is the rigidity modulus of the beam in the axial direction.

$$\frac{d}{dx}\left[EA(x)\frac{dY(x)}{dx}\right] = \omega^2 m(x) Y(x) \tag{4}$$

And the boundary conditions

$$Y(0) = 0 \text{ and}$$

$$EA(x)\frac{dY(x)}{dx}\bigg|_{x=L} = 0$$

Case 2: In this case, the CNT beam is considered as having a rigid mass M. Here also the differential equation remains as same in the form of the case1, the boundary conditions in this case are different.

The differential equation for Eigen value problem is given by

$$\frac{d}{dx}\left[EA(x)\frac{dY(x)}{dx}\right] = \omega^2 m(x)Y(x)$$

$$0 < x < L \tag{5}$$

And the boundary conditions in this case are

$$Y(0) = 0 \text{ and}$$

$$EA(x)\frac{dY(x)}{dx}\bigg|_{x=L} = \omega^2 MY(L)$$

The mass of the nano–particle attached to the CNT at the end and at various intermediate positions is taken to be same.

3. RESULTS AND DISCUSSIONS

In this article, the commercial finite element analysis software package ANSYS has been applied to study the mechanical vibration analysis of the cylindrical shape SWCNTs having with a small thickness. Before considering the suitability of the SWCNT for mass detection applications, it is necessary to verify the accuracy of the finite element model. In this article, the SWCNTs are modeled using a 3D finite element model. The finite element model, used in this article is SOLID 64 to simulate the mechanical vibration response of the SWCNTs.

In this article, the finite element models of the SWCNTs have been analyzed with and without the addition of mass at their ends as well at intermediate positions.

This analysis explores the resonant frequency change caused by the addition of any nano particle at the beam end or at any intermediate positions. The resonant frequency of the carbon nanotube is or higher for the nanotubes having no nano particle at its end or any other intermediate positions. This analysis also indicates that the resonant frequency of the nanotube is going on increasing from the end point to its fixed end position.

In this analysis, we have modeled SWCNTs of cylindrical shapes having small thickness or shell like shapes. Some of the models that have been developed for the purpose of analysis are as follows : (1) The SWCNTs not having any attached mass at their end point or at its intermediate positions is shown in fig. [1 (a)]. (2) The SWCNTs having a nano particle at its end point or any other intermediate positions along its length is shown in fig. [1 (b)]. The finite element models use the anisotropic material properties to simulate the SWCNTs. The tables summarize the simulation results for the first five natural frequencies of the SWCNTs.

Table 1 shows both the numerical and the FEM simulated results for the nanotubes having no attached nano particle on its end or any other position along its length. Table 2 shows the numerical and FEM simulated results of the nanotubes having attached nano particle on its end or tip. It may be observe a that the resonant frequency shift for the nanotubes having attached mass at its end point is reducing comparatively with the nanotubes having no attached mass at its end point. Similarly Tables 3, 4, 5, and 6 shows both the FEM simulated and numerical results of the SWCNTs with attached mass at its free end from 1 μm [1(c)], 2 μm [1(d)], 3 μm [1(e)], and 4 μm [1(f)], respectively. The resonant frequency shift of the nanotubes is continuously increasing when there is a change in the position of the attached mass on the nanotube from its free end.

The change in the resonant frequency is also very small for the nanotube that doesn't have any attached mass at its end point to the nanotube having attached mass at its end point. We can also observe this frequency shift for the nanotubes are having an attached mass along its length at various positions.

The resonant frequency for the SWCNT having the length of 5.5 μm outer radius: 33 nm and Inner radius: 8.8 nm is shown below:

Table 1
The Resonant Frequency Shift for the SWCNT without Attaching Nano–particle on it

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8258243	8589800
f_2	8391121	8687500
f_3	48347915	50547000
f_4	52913421	54265000
f_5	85021920	87509000

Table 2
The Resonant Frequency Shift for the SWCNT with Attached Mass at its End

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8192169	8325200
f_2	7953098	8414600
f_3	48790865	49186000
f_4	51924642	52739000
f_5	81754374	82799000

Table 3
The Resonant Frequency Shift for the SWCNT with Attached Mass at 1μm from its Free End

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8029447	8433600
f_2	8192182	8529700
f_3	49505241	50522000
f_4	53141092	54271000
f_5	81931474	83345000

Table 4
The Resonant Frequency Shift for the SWCNT with Attached Mass at 2 μm from its Free End

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8195098	8519000
f_2	8286097	8614100
f_3	49501972	50239000
f_4	51828623	53963000
f_5	82342768	84555000

Table 5
The Resonant Frequency Shift for the SWCNT with Attached Mass at 3 μm from its Free End

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8254927	8537800
f_2	8346019	8629300
f_3	47996982	49708000
f_4	51930924	53275000
f_5	86082152	88433000

Table 6
The Resonant Frequency Shift for the SWCNT with Attached Mass at 4 μm from its Free End

Resonant frequency(Hz)	*Numerical Result*	*FEM simulated*
f_1	8345921	8602600
f_2	8466902	8701900
f_3	48500972	50174000
f_4	52538723	53920000
f_5	85976426	87712000

The following figures show the finite models of the SWCNT having the length of 5.5μm Outer radius: 33nm, and Inner radius: 8.8nm:

In this section, nano-scale particle is attached to the SWCNTs and the mechanical vibration behavior of the nanotube investigated by means of finite element method analysis. We have developed SWCNTs having different dimensions in terms of various lengths and having various inner and outer diameters. We have investigated the mechanical vibration analysis for all of the nanotubes. Also we have found that the resonant frequency shifts are different for various sizes of the nanotube. This article, presents the numerical and FEM simulated results for the CNT having a 33nm outer radius and 8.8nm inner radius with a length of 5.5μm. It is shown that the finite element method simulation results are in good agreement with the numerical results.

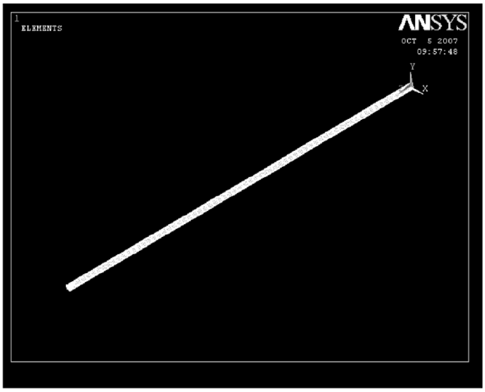

Figure (a): SWCNT Finite Element Model without any Attached Mass

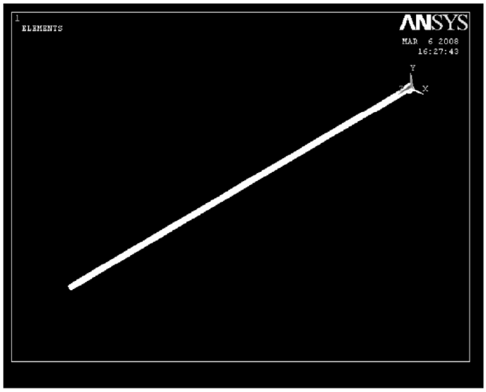

Figure (b): SWCNT Finite Element Model with Attached Mass at its End

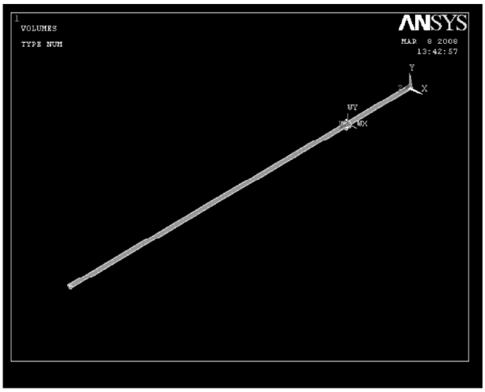

Figure (c): SWCNT Finite Element Model with Attached Mass at 1μm from its Free End

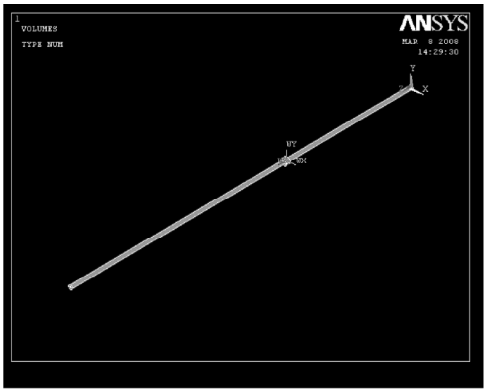

Figure (d): SWCNT Finite Element Model with Attached Mass at 2μm from its Free End

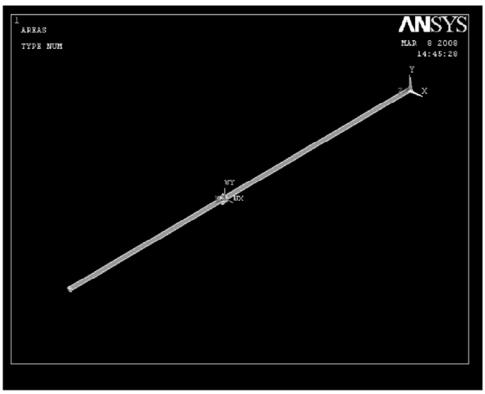

Figure (e): SWCNT Finite Element Model with Attached Mass at 3 μm from its Free End

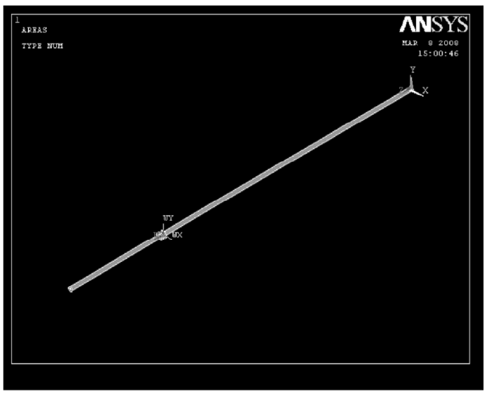

Figure (f): SWCNT Finite Element Model with Attached Mass at 4 μm from its Free End

CONCLUSIONS

(1) The study undertaken in the present work has analyzed the modeling of cantilevered SWCNT using a Finite Element model.

(2) Due to advantages of convenience, rapidity, accuracy, low cost, ease of implementation and ease of use, the finite element method software allows not only the straightforward generation of structural model of a carbon nanotube, but also enables the accurate simulation of its mechanical response. In this study, the resonant frequency analysis of SWCNT has been analyzed using ANSYS.

(3) The addition of the small nano-particle on its length or at its end point or tip offers the potential of meeting the high-performance requirement of many sensing applications, including metal deposition monitors, chemical reaction monitors, biomedical sensors, mass sensors, etc.

(4) The resonant frequency analysis is widely used in small mass detection techniques.

(5) Additionally, this study explores the resonant frequency shift of the SWCNTs caused by the changes in the size of the CNT in terms of length and tube radii.

(6) The results indicate that the mass sensitivity of carbon nanotube – based mass detectors can reach 10^{-21} g and above.

(7) The results of this research work confirm that a SWCNT can be employed as a high precision mass sensor.

References

[1] Huang, S., Cai, X., and Liu. J. "Growth of Millimeter-long and Horizontally Aligned Single-Walled Carbon" *Journal of American Chemical Society*, **125**, 5636–5637, (2003).

[2] Iijima, Sumio "Helical Microtubules of Graphitic Carbon". *International Weekly Journal of Science*, **354**: 56–58, (1991).

[3] Iijima, Sumio "Single-shell Carbon Nanotubes of 1-nm diameter". *International Weekly Journal of Science*, **363**: 603–605, (1993).

[4] H. Dai, J. H. Hafner, A. G. Rinzler, D. T. Colbert, R. E. Smalley, *"Nanotubes as Nanoprobes in Scanning Probe Microscopy."* Sensors and Actuators A: Physical, **384**: 147–150, (1996).

[5] P. Poncharal, Z. L. Wang, D. Ugarte, W. A. D. Heer, *"Electrostatic Deflections and Electro-mechanical Resonances of Carbon Nanotubes."* Science Magazine, AAAS, **283**: 1513–1516. (1999).

[6] H. J. Qi, K. B. K. Teo, K. K. S. Lau, M. C. Boyce, W. I. Milne, J. Roberson, K. K. Gleason, "Determination of Mechanical Properties of Carbon Nanotubes and Vertically Aligned Carbon Nanotube Forests using Nanoindentation" *Journal of the Mechanics and Physics of Solids*, **51**: 2213-2237. (2003).

[7] G.W. Wang, Y. P. Zhao, G. T. Yang, "The Stability of a Vertical Singlewalled Carbon Nanotube under its Own Weight." *Materials & Design*, **25**: 453–457, (2004).

[8] R. Mateiu, Z. J. Davis, D. N. Madsen, K. Molhave, P. Boggild, A. M. Rassmusen, M. Brorson, C. J. H. Jacobsen, and A. Boisen. "An Approach to a Multi-walled Carbon Nanotube based Mass Sensor". *Microelectronic Engineering*, C 23-24, pp. 670-674, (2004).

[9] C. J. Brabec, A. Maiti, C. Roland, J. Bernholc, "Growth of Carbon Nanotubes—A Molecular Dynamics Study" *Chemical Physics Letters.*, **236**: 150–155, (1995).

[10] C. Mak and J. Krim "Quartz-crystal Microbalance Studies of the Velocity Dependence of Interfacial Friction" *Physical Review Letters B.*, **58**, [9], (1998).

[11] E. Benes, M. Groschl, W. Burger and M. Schmid, "Sensors based on Piezoelectric Resonators", *Sensors and Actuators A (Phys.)* **48**: 1–21, (1995).

[12] T. Thundat, P. I. Oden and R. J. Warmack, *"Microcantilever sensors"*, Microscale Thermophys. Eng. **1**: 185–199, (1997).

[13] P. Hauptmann, R. Lucklum, A. Puttmer and B. Henning, "Ultrasonic Sensors for Process Monitoring and Chemical Analysis" *Sensors and Actuators A* **67**: 32-36, (1998).

[14] Q. S. Zheng and Q. Jiang, "Multiwalled Carbon Nanotubes as Gigahertz Oscillators", *Physical Review Letters,* **8** [4]: 455-503, (2002).

[15] Philip Kim and Charles M. Lieber "Nanotube Nanotweezers" *Science Magazine, AAAS*, **286,** [5447], 2148–2150, (1999).

APPENDIX: MATERIAL PROPERTIES OF CNTS

The young's modulus: 1.2 Tpa

Density: 1330 kg/m^3.

Stiffness (multiplied by 10^9)	
c_{11}	1060
c_{12}	15
c_{13}	180
c_{14}	0
c_{15}	0
c_{16}	0
c_{22}	36.5
c_{23}	15
c_{24}	0
c_{25}	0
c_{26}	0
c_{33}	1060
c_{34}	0
c_{35}	0
c_{36}	0
c_{44}	2.25
c_{45}	0
c_{46}	0
c_{55}	220
c_{56}	0
c_{66}	2.25