

## Modeling of carbon nanotubes (CNTs) and usage in drug delivery.

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### **Abstract.**

One goal of device science is miniaturization; hence nanotechnology has received considerable attention. The possibility that the unique properties of nanostructures will result in novel applications and devices is an enticing goal. Carbon nanotubes are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with a length-to-diameter ratio of up to 28,000,000:1. Potential applications for carbon nanotubes (CNTs) include their use in atomic force microscopy and in adhesives, certainly chemical or mathematical investigation of nanotubes is very important but investigates both of them together has vital notability. there is considerable open literature related to the mathematical modeling of nanotubes, also many authors have investigated the chemical aspects of nanotubes. At the present, in this review, my aim is to both mathematical and chemical aspects of structured, characteristics are investigated.

**Keywords:** nanotube, MWNT, isotropic, mathematical model.

### **1-Introduction:**

Carbon nanotubes, long, thin cylinders of carbon, were discovered in 1991 by S. Iijima. These are large macromolecules that are unique in their size, shape, and remarkable physical properties. They can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into a cylinder. These intriguing structures have sparked much excitement in recent years and a large amount of research has been dedicated to their understanding. Currently, the physical properties are still being discovered and disputed. What makes it so difficult is that nanotubes have a very broad range of electronic, thermal, and structural properties that change depending on the different kinds of nanotubes (defined by its diameter, length, or twist). To make things more interesting, besides having a single cylindrical wall (SWNTs), nanotubes can have multiple walls (MWNTs)--cylinders inside the other cylinders.

### **2-Mathematical aspect:**

Equations for transversely isotropic linearly elastic materials:

Transversely isotropic materials are those materials that possess a single axis about which the material is isotropic, but the material is not isotropic with respect to any other axis. In other words, transversely isotropic materials have the same properties in a plane which orthogonal to the single axis, but these properties differ for different planes along the axis. This constitutive assumption has been proposed for carbon nanotubes [16]. However, not all authors adopt this approach. We can show that both the inner

and outer tubes, as rolled graphite monolayers, can be successfully modeled as thin shells with an extremely high in- shell Young's modulus (E= 5.5 TPa) and an extra-thin thickness (h= 0.067 nm). If the carbon nanotubes are modeled as a thick tube of transversely isotropic material, then this could result in illusive interior vibrations. From the stress and strain relations as given by Hooke's law, we may write the stiffness matrix in the form:

$$\begin{matrix}
 \sigma_{xx} & & C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
 \sigma_{yy} & & C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
 \sigma_{zz} & = & C_{11} & C_{12} & C_{33} & 0 & 0 & 0 \\
 \sigma_{yz} & & 0 & 0 & 0 & 2C_{44} & 0 & 0 \\
 \sigma_{zx} & & 0 & 0 & 0 & 0 & 2C_{44} & 0 \\
 \sigma_{xy} & & 0 & 0 & 0_3 & 0 & 0 & C_{11} - C_{12}
 \end{matrix} \tag{1}$$

where C<sub>kl</sub> (k, l = 1,2,3,4) denote certain constants, C<sub>ij</sub> (i, j = 1,2,3) denote the Cauchy stress tensor in Cartesian coordinates x<sub>j</sub> (j = 1,2,3) = (x, y, z) and we adopt the strain tensor defined by:

$$\epsilon_{ii} = \frac{1}{2} \left( \frac{\delta u_i}{\delta x^j} + \frac{\delta u_j}{\delta x^i} \right), \quad (i, j = 1, 2, 3) \tag{2}$$

Where u<sub>i</sub> (x, y, z) (i = 1, 2, 3) denote the three displacements (u, v, w). Explicitly in terms of (x,y, z) we have

$$\epsilon_{xx} = \frac{\delta u}{\delta x}, \quad \epsilon_{yy} = \frac{\delta v}{\delta y}, \quad \epsilon_{zz} = \frac{\delta w}{\delta z}, \quad \epsilon_{yz} = \frac{1}{2} \left( \frac{\delta v}{\delta z} + \frac{\delta w}{\delta y} \right), \quad \epsilon_{zx} = \frac{1}{2} \left( \frac{\delta w}{\delta x} + \frac{\delta u}{\delta z} \right), \quad \epsilon_{xy} = \frac{1}{2} \left( \frac{\delta u}{\delta y} + \frac{\delta v}{\delta x} \right) \tag{3}$$

And this notation is adopted by, Sokolnikoff. We emphasize that some authors employ the notation referred to as the engineering strain

$$\epsilon_{xx} = \frac{\delta u}{\delta x}, \quad \epsilon_{yy} = \frac{\delta v}{\delta y}, \quad \epsilon_{zz} = \frac{\delta w}{\delta z}, \quad \epsilon_{yz} = \frac{1}{2} \left( \frac{\delta v}{\delta z} + \frac{\delta w}{\delta y} \right), \quad \epsilon_{zx} = \frac{1}{2} \left( \frac{\delta w}{\delta x} + \frac{\delta u}{\delta z} \right), \quad \epsilon_{xy} = \frac{1}{2} \left( \frac{\delta u}{\delta y} + \frac{\delta v}{\delta x} \right) \tag{4}$$

$$e_{xx} = \frac{\delta u}{\delta x}, \quad e_{yy} = \frac{\delta v}{\delta y}, \quad e_{zz} = \frac{\delta w}{\delta z}, \quad e_{yz} = \left( \frac{\delta v}{\delta z} + \frac{\delta w}{\delta y} \right), \quad e_{zx} = \left( \frac{\delta w}{\delta x} + \frac{\delta u}{\delta z} \right), \quad e_{xy} = \left( \frac{\delta u}{\delta y} + \frac{\delta v}{\delta x} \right) \tag{5}$$

$$\begin{array}{ccccccc}
 \epsilon_{XX} & S_{11} & S_{12} & S_{13} & 0 & 0 & 0 & \sigma_{XX} \\
 \epsilon_{YY} & S_{12} & S_{11} & S_{13} & 0 & 0 & 0 & \sigma_{YY} \\
 \epsilon_{ZZ} & S_{13} & S_{13} & S_{33} & 0 & 0 & 0 & \sigma_{ZZ} \\
 \epsilon_{YZ} & 0 & 0 & 0 & S_{44/2} & 0 & 0 & \sigma_{yz} \\
 \epsilon_{ZX} & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{zx} \\
 \epsilon_{XY} & 0 & 0 & 0_3 & 0 & 0 & S_{11} - S_{12} & \sigma_{xy}
 \end{array} \quad (6)$$

In terms of the Poisson’s ratio and Young’s modulus in the transverse plane and Poisson’s ratio, Young’s modulus and shear modulus in the longitudinal directions; namely  $\nu, E$ , and  $\nu, E, \mu$ , respectively, we have the relations

$$\begin{aligned}
 \epsilon_{xx} &= \frac{1}{E} (\delta_{xx} - \nu \delta_{yy}) - \frac{\nu'}{E'} \delta_{zz} & \epsilon_{xz} &= \frac{1}{2\mu'} \delta_{xz} \\
 \epsilon_{yy} &= \frac{1}{E} (-\nu \delta_{xx} - \delta_{yy}) - \frac{\nu'}{E'} \delta_{zz} & \epsilon_{yz} &= \frac{1}{2\mu'} \delta_{yz} \\
 \epsilon_{zz} &= \frac{\nu'}{E'} (\delta_{xx} + \delta_{yy}) + \frac{1}{E} \delta_{zz} & \epsilon_{xy} &= \frac{1+\nu}{E} \delta_{xy}
 \end{aligned} \quad (7)$$

And the following values for the constants  $S_{ij}$  can be written as:

$$S_{11} = \frac{1}{E}, \quad S_{12} = -\frac{\nu}{E}, \quad S_{13} = -\frac{\nu'}{E'}, \quad S_{44} = \frac{1}{E'} \quad (8)$$

The constants  $C_{ij}$  can be shown to be given by the expressions:

$$C_{11} = -\Delta^* \frac{(E\nu'^2 - E')}{1+\nu}, \quad C_{12} = -\Delta^* \frac{E\nu - E\nu'^2}{1+\nu}, \quad C_{13} = -\Delta^* E\nu' \quad (9)$$

$$C_{33} = \Delta^* \frac{E^2}{E} (\nu - 1), \quad C_{33} = \mu'$$

Where the quantity  $\Delta^*$  is defined by:

$$\Delta^* = \frac{E}{E\nu - E' + 2E\nu'^2} \quad (10)$$

We note that in cylindrical coordinates (r, h, z) the stiffness matrix involves the same constants as in Cartesian coordinates and is given by:

$$\begin{matrix}
 \sigma_{rr} & & C_{11} & C_{12} & C_{13} & 0 & 0 & 0 & \varepsilon_{rr} \\
 \sigma_{\theta\theta} & & C_{11} & C_{12} & C_{13} & 0 & 0 & 0 & \varepsilon_{\theta\theta} \\
 \sigma_{zz} & = & C_{11} & C_{12} & C_{33} & 0 & 0 & 0 & \varepsilon_{zz} \\
 \sigma_{\theta z} & & 0 & 0 & 0 & 2C_{44} & 0 & 0 & \varepsilon_{\theta z} \\
 \sigma_{rz} & & 0 & 0 & 0 & 0 & 2C_{44} & 0 & \varepsilon_{rz} \\
 \sigma_{r\theta} & & 0 & 0 & 0 & 0 & 0 & C_{11} - C_{12} & \varepsilon_{r\theta}
 \end{matrix} \quad (11)$$

Further, in cylindrical polar coordinates (r, h, z), the momentum equations can be written in vector form as the following:

$$\begin{aligned}
 & \frac{\delta\sigma_{rr}}{\delta r} + \frac{1}{r} \frac{\delta\sigma_{r\theta}}{\delta\theta} + \frac{\delta\sigma_{r\theta}}{\delta\theta} + \frac{\delta\sigma_{rz}}{\delta z} + \frac{\delta r r - \delta\theta\theta}{r} + f_r = \rho \frac{d^2u}{dt^2} \\
 & \frac{\delta\sigma_{r\theta}}{\delta r} + \frac{1}{r} \frac{\delta\theta\theta}{\delta\theta} + \frac{\delta\sigma_{r\theta}}{\delta\theta} + \frac{\delta\sigma_{\theta z}}{\delta z} + \frac{2}{r} \sigma_{r\theta} + f_{\theta} = \rho \frac{d^2v}{dt^2} \\
 & \frac{\delta\sigma_{rz}}{\delta r} + \frac{1}{r} \frac{\delta\theta z}{\delta\theta} + \frac{\delta\sigma_{\theta z}}{\delta\theta} + \frac{\delta\sigma_{\theta z}}{\delta z} + \frac{1}{r} \sigma_{rz} + f_z = \rho \frac{d^2w}{dt^2}
 \end{aligned} \quad (12)$$

After similar calculations, from these relations, the momentum Eq. (12) for transversely isotropic linearly elastic materials can be written as:

$$\begin{aligned}
 & \frac{(C_{11} - C_{12})}{2} \frac{1}{r^2} \frac{\delta^2 u}{\delta\theta^2} + C_{44} \frac{\delta^2 u}{\delta z^2} + \frac{(C_{11} + C_{12})}{2} \frac{1}{r} \frac{\delta^2 u}{\delta r \delta\theta} - C_{11} \frac{1}{r^2} + (C_{13} + C_{44}) \frac{d^2 w}{\delta r \delta z} + \\
 & C_{11} \frac{1}{r} \frac{\delta u}{\delta r} - \frac{(3C_{11} - C_{12})}{2} + \frac{1}{r^2} \frac{\delta v}{\delta r \delta\theta} + f_r = \rho \frac{d^2 u}{dt^2} \\
 & \frac{(C_{11} - C_{12})}{2} \frac{\delta^2 v}{\delta r^2} + C_{11} \frac{1}{r^2} \frac{\delta^2 v}{\delta\theta^2} + C_{44} \frac{d^2 v}{d\theta^2} + \frac{(C_{11} + C_{12})}{2} \frac{1}{r} \frac{\delta^2 u}{\delta r \delta\theta} + (C_{13} + C_{44})
 \end{aligned}$$

$$\frac{1}{r} \frac{\delta^2 w}{\delta z \delta \theta} + \frac{(3C_{11} - C_{12})}{2} \frac{1}{r^2} \frac{\delta u}{\delta \theta} + \frac{(C_{11} - C_{12})}{2} \frac{1}{r} \frac{\delta v}{\delta r} - \frac{(C_{11} - C_{12})}{2} \frac{1}{r^2} v + f_{\theta} = \rho \frac{d^2 v}{dt^2}$$

$$C_{44} \frac{\delta^2 w}{\delta r} + C_{44} \frac{1}{r^2} \frac{\delta^2 w}{\delta \theta^2} + C_{33} \frac{\delta^2 w}{\delta z^2} + (C_{13} + C_{44}) \frac{\delta^2 u}{\delta r \delta z} + (C_{13} + C_{44})$$

$$\frac{1}{r} \frac{\delta^2 v}{\delta z \delta \theta} + (C_{13} + C_{44}) \frac{1}{r} \frac{\delta u}{\delta z} + C_{44} \frac{1}{r} \frac{\delta w}{\delta r} + f_z = \rho \frac{d^2 w}{dt^2} \tag{13}$$

Where Ckl are the constants appearing in Hooke’s law as given by Eq. (1).

**3-chemical aspect:**

Since the discovery of carbon nanotubes [1, 2], they have attracted much attention because of their unique properties that may impact many fields of science and technology [3–6]. Much research has been done for their synthesis, and several methods such as electric arc discharge, laser ablation laser ablation, and catalytic decomposition of hydrocarbons [7] have been established. Among these methods, we believe that the catalytic method would be the most efficient for large-scale and low-cost synthesis. For example, Pd-CNT catalyst for hydro dehalogenation of aryl halides, Pd- CNT for hydrazine oxidation, Pt-CeO2/CNT for methanol electro-oxidation and etc. in this part we chose Dual-catalyst growth of vertically aligned carbon nanotubes at low temperature in thermal chemical vapor deposition [8] In the growth of carbon nanotubes (CNTs), several methods have been employed such as laser vaporization [9], arc discharge [10], and chemical vapor deposition (CVD) [11,12]. Laser vaporization and arc discharge methods are advantageous for the growth of the highly purified CNTs but are difficult to control the CNTs during growth because of high-growth temperature. On the other hand, the CVD method has been successful to produce the CNTs in large quantities, and also to obtain the vertically aligned CNTs at relatively low temperatures. In particular, the growth of vertically aligned CNTs on a large substrate area at low temperature, for instance, softening temperature of the glass is an important factor for the practical structure of Emitters to the field emission displays [13] Because the melting temperature of the soda–lime glass, which is commonly used as a substrate, is about 550 \_C, it is necessary to grow the CNTs on the soda–lime glass using the thermal CVD than other methods. Recently, we succeeded to synthesize the CNTs at low temperatures below 550\_C using plasma-enhanced CVD (PECVD) [14]. However, the CNT growth on a large substrate area is not easily accessible with the PECVD method because of the limitation of the plasma area. Although thermal CVD provides a way to grow CNTs in a large area, lowering the growth temperature to a practical level cannot be easily achieved with a conventional approach. Therefore, it is essential to reduce the growth temperature to a glass softening temperature or even below, if possible. Although MWNTs were discovered first, multi-walled carbon nanotubes (MWNTs) have not been studied as thoroughly as single-walled carbon nanotubes (SWNTs). This could partly be due to the higher specific stiffness and strength of an SWNT as compared to those of an MWNT. However, in certain applications, MWNTs offer superior properties over SWNTs.

#### 4-Application of carbon nanotubes in medicine filed

Lung cancer is one of the most prevalent cancers and the leading cause of death worldwide. In this study, a specific agonist of DRDs, BRC was delivered to lung cancer cells with MWCNTs and showed a significant anti-proliferative effect on cancer cells and low toxicity on normal lung cells [18]. Furthermore, one of these fundamental variables is the blood glucose level of a diabetic person. However similar to most artificial control systems associated with the human body, many complexities and uncertainties force us to use advanced control methods. In this paper, by choosing a successfully applied model, a nonlinear controller and observer are designed to control blood glucose levels. This mathematical model, which is called Bergman minimal model, approximates the dynamic reaction of a diabetic patient's blood glucose concentration to the insulin injection. These equations are non-normal nonlinear with some uncertainties. The backstepping method is applied to control the system due to its non-normal equations.[19] It is widely accepted that supercritical fluids (SCF) pose some valuable advantages over traditional solvents (liquid-like density, gas-like transport properties, low surface tension, and good mass transfer capacity). These characteristics have drawn attention to the SCFs as solvent media for supercritical extraction/purification purposes in a wide range of applications<sup>1</sup>. Carbon dioxide (CO<sub>2</sub>) is likely the most trustful supercritical fluid in energy, food, pharmaceutical, and bioactive agent delivery applications. Indeed, the non-toxic, inflammable, and non-explosive nature of supercritical carbon dioxide (SCCO<sub>2</sub>) is responsible for this trustful applications<sup>2</sup>. Furthermore, the SCCO<sub>2</sub> critical characteristics are mild (temperature = 31.1 °C, pressure = 73.8 bar), it is recyclable, simply available at low expense, and covers the real-field requirement.[29]. Using medicines that used CNT technology may be related to increase force production and neural adaptation. The usage of glycolytic pathways, which results in a rise in the concentration of phosphofructokinase or phosphorylase enzymes and a consequent relative increase in force generation and brain adaptation, are among the mechanisms that may be responsible for enhancing anaerobic power.[30]. Clinical translation of cell therapies requires strategies that can manufacture cells efficiently and economically. One promising way to reproducibly expand T cells for cancer therapy is by attaching the stimuli for T cells onto artificial substrates with high surface area. A carbon nanotube-polymer composite can act as an artificial antigen-presenting cell to efficiently expand the number of T cells isolated from mice. We attach antigens onto bundled carbon nanotubes and combined this complex with polymer nanoparticles containing magnetite and the T-cell growth factor interleukin-2 (IL-2). The number of T cells obtained was comparable to clinical standards using a thousand-fold less soluble IL-2. T cells obtained from this expansion were able to delay tumor growth in a murine model for melanoma. Our results show that this composite is a useful platform for generating large numbers of cytotoxic T cells for cancer immunotherapy.[31]

On the other hand, nobody can deny the downsides of CNT on health. Anthropogenic carbon nanotubes, with a fibrous structure and physical properties similar to asbestos, have recently been found within human lung tissues. However, the reported carbon-nanotube-elicited pulmonary pathologies have been mostly confined to inflammatory or neoplastic lesions in the lungs or adjacent tissues. It could be demonstrated that demonstrate that a single pulmonary exposure to multi-walled carbon nanotubes dramatically enhances angiogenesis and the invasiveness of orthotopically implanted mammary carcinoma, leading to metastasis and rapid colonization of the lungs and other organs. Exposure to multi-walled carbon nanotubes stimulates local and systemic inflammation, contributing to the formation of pre-metastatic and metastatic niches. Our study suggests that nanoscale-material-elicited pulmonary lesions may exert complex and extended influences on tumor progression. Given the increasing presence of carbon nanotubes in the environment,

this report emphasizes the urgent need to escalate efforts in assessing the long-term risks of airborne nanomaterial exposure in non-lung cancer progression.[20]. single-walled CNT and to a lesser extent multi-walled and its COOH-functionalized form induced CAF-like cells, which are non-tumorigenic in animals, but promote tumor growth of human lung carcinoma and CNT-transformed lung epithelial cells. The mechanism by which CNT-induced CAF-like cells promote tumor growth involved the acquisition of cancer stem cells (CSCs) in the cancer population. Gene knockdown experiments showed that an expression of podoplanin on CAF-like cells is essential for their effects, indicating the functional role of CAF-like cells and podoplanin in the CNT tumorigenic process. Our findings unveil a novel mechanism of CNT-induced carcinogenesis through the induction of CAF-like cells that support CSCs and drive tumor formation. Our results also suggest the potential utility of podoplanin as a mechanism-based biomarker for rapid screening of carcinogenicity of CNTs and related nanomaterials for their safer design.[21] In 1958, it was introduced as a herbicide for dicotyledons<sup>3</sup>. Due to biodegradation by microbes, the half-life time of ATZ in the soil is 261 days, whereas degradation takes longer in water due to low solubility [22,23] Consumption of ATZ-rich water causes several health problems such as endocrine disruption and hormone disruption, with the risk of breast and prostate cancer [25],[26],[27]. Notably, children are the most adversely affected. Further, exposure to ATZ during the maternity period results in low fetal weight and limb/urinary/heart defects, with the risk of reduced survival on prolonged exposure to high-level concentrations. According to the US environmental protection agency, the maximum acceptable level of ATZ concentration in drinking water is 3 parts per billion<sup>9</sup>, although long-term exposure to such low concentrations also affects the human endocrine system severely. On account of the adverse effects of ATZ on the environment, it is desirable to develop biosensor platforms that can detect the same in water, both qualitatively and quantitatively.[28]

#### 4-Conclusions:

As we have seen in the mathematical modeling part, we presume that external tubs remain to fix therefore, we can model and similarities as transversely isotropic linearly elastic materials and oscillation inner tube of double-walled carbon nanotubes, we analyze this modeling with the investigated categorization of Nanotubes as single-walled (SWNTs) and multi-walled (MWNTs), we have studied a summary of produce nanotubes unusual methods, as arc discharge or laser ablation. Using of CNTs in improving drug and medicine delivery has a great effect on medical technology. According to our research, SWNTs increase the solubility of drugs and enhance the targeting of tumors. As a drug delivery vehicle, Carbon nanotubes', pave the way for targeting cancer cells with a lower dosage rather than common drugs. Although CNTs have a lot of positive effects on people's health by using them as a useful medical vehicle, we should not deny the downside of CNTs can lead to inflammatory or neoplastic lesions in the lungs or adjacent tissues.

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