International Journal of Smart Energy Technology and Environmental Engineering
Volume 3, Issue 1, March 2024
https://setee.globalpublisher.org/
http://globalpublisher.org/journals-1007/

Vibrations of single-walled carbon nanotubes: a novel method for delivering anti-cancer drugs

Fatemeh Mojaver[1], Seyedeh Mahsa Zarei[1], Negar Salmani[1] , Hassan Ghalami Bavil Olyaee[2,*]
1- Ph.D. Student, Medical Engineering - Department of Advanced Medical Sciences and Technologies, Faculty of Engineering, Islamic Azad University, South Tehran Branch, Tehran, Iran.
2- Assistant Professor, Physics - Department of Basic Sciences, Faculty of Engineering, Islamic Azad University, South Tehran Branch, Tehran, Iran
*Corresponding Author: Olyaee@azad.ac.ir

ABSTRACT

In this paper, we conduct a meticulous investigation into the oscillations of single-walled carbon nanotubes (SWCNTs) and their consequential effects on drug delivery methodologies and cancer therapeutics. Owing to their distinctive electronic characteristics, carbon nanotubes have captured significant interest and have been utilized across diverse domains, including the fabrication of sensors, thermal conduction, composite materials, and medical applications. This research scrutinizes the physical attributes of carbon nanotubes and then assesses their role in the realm of cancer treatment. Employing the Galerkin method, we model and analyze the oscillatory behavior of carbon nanotubes under the influence of external forces within a context pertinent to drug conveyance. Additionally, non-local elasticity theory is applied to articulate the behavior of these nanocarbon tubes. The outcomes of this study suggest that the application of carbon nanotubes can positively influence the absorption and permeability of cancerous cells, thereby augmenting the effects of cytotoxicity and therapeutic efficacy. This novel amalgamation could be adopted as an innovative and effective approach in the fight against cancer. The research undertaken herein has the potential to contribute to the advancement of more sophisticated treatment modalities, ultimately leading to an enhancement in the quality of life for individuals afflicted with cancer. This study, with its emphasis on the importance of carbon nanotubes within contemporary therapeutic strategies, marks a pivotal stride in propelling the knowledge of nanomedical science and proffering targeted, minimally invasive treatment options. The examinations conducted in this article hold promise not only for cancer therapy but also for future breakthroughs in nanomedicine.

Keywords: CNT, Vibration, drug delivery, cancer therapy, Galerkin method, nonlocal elasticity theory

1. INTRODUCTION

This paper investigates the physical and vibrational properties of single-walled carbon nanotubes (SWCNTs) on drug delivery and cancer treatment. Cancer is a dangerous and complex disease that occurs widely around the world and has caused significant mortality. In recent years, many efforts have been made to develop new and effective treatment methods for cancer.

Research on the use of carbon nanotubes in cancer treatment began in the 2000s. Studies have shown that carbon nanotubes act as an effective drug carrier for precise delivery of drugs to cancer cells [1]. Sun and colleagues discuss two methods of using single-walled carbon nanotubes for delivering anti-cancer drugs, namely physical and chemical methods. Also, the biological effects and toxicities associated with the use of these nanotubes are investigated [2]. Chen and colleagues use single-walled carbon nanotubes to deliver anti-cancer drugs for cancer treatment in laboratory animals. The experimental results show that the use of this method can have a significant improvement in the efficacy of cancer treatment [3]. Pantarotto and colleagues use single-walled carbon nanotubes to deliver genes to cells. The biological effects and cellular tolerance of these nanotubes are also investigated [4]. Zhang and colleagues investigate the use of carbon nanotubes as a drug delivery system in anti-cancer treatments. Carbon nanotubes, due to their unique physical and chemical properties, can deliver drugs effectively and selectively and increase the therapeutic efficacy [5]. Kim and colleagues investigate how carbon nanotubes can be used, in addition to delivering drugs to cancer cells, as a near-infrared agent for targeted destruction of cancer cells [6]. Chen and colleagues investigate the use of carbon nanotubes for drug delivery in cancer treatment in live animals. The research shows that carbon nanotubes can be used as an effective mediator for drug delivery in cancer treatment and improve the therapeutic efficiency [7]. Leo and colleagues investigate the use of carbon nanotubes for delivering nucleic acids and genes in gene therapy. Carbon nanotubes, due to their high transport power and ability to stimulate the immune system in the body, can be used to deliver nucleic acids and genes to cells [8]. Winters and colleagues investigate the use of carbon nanotubes as a mediator for delivering short interfering RNA (siRNA) to new combinations of human T cells and primary cells. The results indicate that carbon nanotubes can be effectively used to deliver siRNA to living cells [9]. Sun and colleagues investigate how supramolecular chemistry on water-soluble carbon nanotubes can help drug tolerance and delivery in cells. Carbon nanotubes are used as an attractive mediator for stabilizing drugs and delivering them to target cells [10]. Leo and colleagues investigate the in vivo distribution and high targeting in tumors by carbon nanotubes in mice. The results show that carbon nanotubes can be effectively used for drug delivery to tumors and cancer treatment [11]. Jin and colleagues investigate the multifunctional carbon nanostructures for medical applications. Carbon nanostructures are used as drug carriers, imaging and cancer treatment [12]. Bianco and colleagues investigate how carbon nanotubes can function in drug delivery to cells and tissues. Carbon nanotubes are used as drug carriers, drug delivery in target cells and tissues and improving therapeutic efficiency [13]. Sun and colleagues investigate the use of graphene oxide nanosheets for cellular imaging and drug delivery. The results show that graphene oxide nanosheets can be effectively used for drug delivery to cells and cellular imaging [14]. Pantarotto and colleagues investigate the transfer of active peptides through cell membranes by carbon nanotubes. The results indicate that carbon nanotubes can be used as a mediator for delivering active peptides to cells [15]. Leo and colleagues provide a comprehensive review of the applications of carbon nanotubes in the field of biology and medicine. This paper discusses intracellular and extracellular imaging, drug delivery and other applications of carbon nanotubes in biology and medicine [16]. Kim and colleagues investigate the use of carbon nanotubes as intracellular protein carriers. The results show that carbon nanotubes can be used as a device for delivering proteins to cells [17].

One of the novel and promising methods in cancer treatment is the use of nanoparticles as a drug carrier. Nanoparticles, due to their special properties and drug delivery power, have been proposed as a suitable platform for delivering anti-cancer drugs to the required areas in cancer. In this regard, carbon nanotubes, as one of the most important carbon nanomaterials, have unique mechanical, electrical, thermal and optical properties that can be used in various applications such as sensors, heat transfer, composites and medicine. In addition, carbon nanotubes, due to their unique physical and electronic properties, improve the ability to have a high surface absorption and distribution of drugs.

To investigate the physical and vibrational properties of carbon nanotubes, the Galerkin method is used, which is a numerical method for solving differential and difference equations. In this method, the problem is decomposed into a space of functions and then using a space of test functions, the differential and difference equations are converted into a series of algebraic equations. Then, using various mathematical techniques, these algebraic equations are solved to obtain an approximation of the exact solution of the problem. Also, the nonlocal elasticity theory is used to describe the behavior of nanotube carbon tubes. This theory in classical continuum mechanics, relates the stress state at a point to the strain distribution in the vicinity of that point. The use of this theory in various fields of nanomechanics, such as scattering and wave propagation, stress mechanics, fracture mechanics and fluids with surface pressure, has been successful. Finally, the Euler-Bernoulli beam model is used to describe the vibrational behavior of carbon nanotubes. This model is one of the simple and common models for analyzing the vibrations of beams and cylinders, which assumes that the transverse deformation of the beam is linearly related to its bending curvature. The boundary conditions used in this paper are Double Simply-supported and Clamped Simply-supported. To solve the equations, Mathematica software is used. Mathematica is a powerful computational software that has the ability to perform mathematical calculations, data analysis, algorithm development, simulations and visualizations.

Translate this text to English: According to the results of this study, it can be concluded that CNT has the highest amplitude of vibration at the lowest critical speed, therefore it can be effective in cancer treatment. This paper shows that CNT can be used as a carrier for delivering anti-cancer drugs to cancer cells and by creating vibrations in them, it causes their death. This treatment method has advantages such as reducing side effects, increasing drug efficacy, reducing treatment costs and improving the quality of life of patients. Of course, this treatment method still needs more studies and clinical trials to be used as a valid and reliable treatment method.

2. Experimental Activities

2.1 Materials and Methods

The aim of this paper is to investigate the vibrations of single-walled carbon nanotubes (SWCNTs) in the presence of external forces and in an environment related to drug delivery. Carbon nanotubes, as one of the most important carbon nanomaterials, have unique mechanical, electrical and thermal properties that can be used in various applications such as sensors, heat transfer, composites and medicine. The vibrations of carbon nanotubes can have a direct impact on their physical properties and performance and should be accurately modeled and analyzed. To model the vibrations of carbon nanotubes, the Galerkin-DQ method is used, which is a numerical method for solving differential and difference equations. This method is used to solve differential and difference problems in various fields such as engineering, physics, mathematics and computer science. In the Galerkin-DQ method, the problem is decomposed into a space of functions and then using a space of test functions, the differential and difference equations are converted into a series of algebraic equations. This space of test functions is usually chosen from basis functions or special functions. Then, using different mathematical techniques, these algebraic equations are solved to obtain an approximation of the exact solution of the problem. This method is usually used as an approximate method for solving differential and difference equations and can be widely used in various problems such as statics, dynamics, heat and fluid flow.

This paper is about the use of nonlocal elasticity theory to analyze the behavior of nanotube carbon tubes (CNTs). This theory in classical continuum mechanics, assumes that the stress state at a point depends on the strain distribution in the vicinity of that point. The use of this theory in various fields of nanomechanics, such as scattering and wave propagation, stress mechanics, fracture mechanics and fluids with surface pressure, has been successful.

2.2. Mathematical modeling

In this paper, we consider carbon nanotubes as a thin and elastic cylinder and use the Euler-Bernoulli beam model to describe their vibrational behavior. This model is one of the simple and common models for analyzing the vibrations of beams and cylinders, which assumes that the transverse deformation of the beam is linearly related to its bending curvature.

2.3 Delivery mechanism

Single-walled carbon nanotubes have great potentials for applications. CNTs are used as a device for transporting and transforming drugs, so that antibodies are placed on them without toxic effects. In addition, fullerene C60 can be considered as nanoparticles. Previous studies have shown that due to the van der Waals interaction between the inner surface of CNT and the fullerene molecule, the C60 molecule, which is at a short distance from the inner surface of the nanotube, is absorbed into the nanotube and starts to oscillate spontaneously. Also, according to figure (1), It is also assumed that the moving nanoparticle with mass m and constant speed v moves along the centerline of CNT. The van der Waals interaction is modeled by linear spring forces that act on CNT in the transverse direction. The nanotube is on an elastic base with a uniform stiffness distribution along CNT. And its initial conditions are assumed to be zero. When a nanoparticle enters a CNT, interactions at the nanoscale occur due to potential fields and external forces on CNT cause vibration in the structure. This model can be extended to study nanodrugs and their delivery.

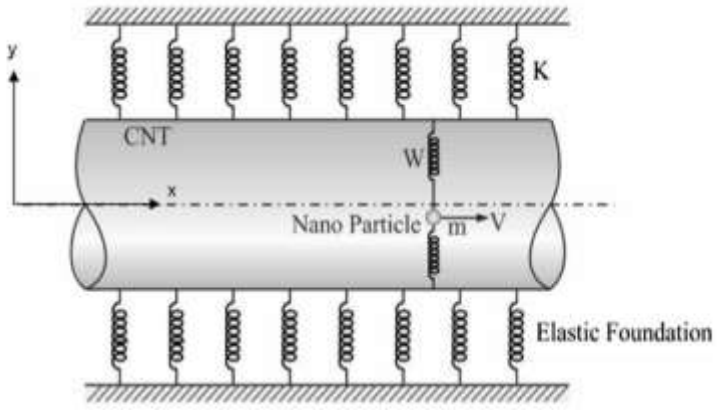

Fig.1. illustrates a schematic view of a single-walled carbon nanotube (CNT) positioned on an elastic foundation alongside a moving nanoparticle.

2.4 Governing equation

"In this paper, we investigate the governing equation of CNT, which includes the governing equation (1) and the dimensionless governing equation (2) for modeling the interaction between a nanoparticle inside the nanotube and an elastic base using the nonlocal Euler-Bernoulli beam theory. In equation (1), different terms involving partial derivatives, stiffness and van der Waals force are used to model the vibration of the nanotube and the nanoparticle. Also, the dimensionless equation (2) is used to model the dimensionless state of the interaction between the nanoparticle and the nanotube." We assume that in the CNT equation, a nanoparticle with mass m moves inside it at a constant speed v. The van der Waals force is modeled as a spring with stiffness W and the surrounding environment is replaced by an elastic base with stiffness K. In addition, the deflection of CNT is modeled as Y(x,t). Here, δ' denotes the derivative of the Dirac delta function with respect to x. Now we can state the governing equation in a simple form.

$$EI\frac{\partial^4 Y}{\partial x^4}+\left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\left[m_c\frac{\partial^2 Y}{\partial t^2}+KY-(mg-WY)\delta(x-vt)\right]=0. \tag{1}$$

$$16\frac{\partial^4\psi}{\partial\xi^4}+\left(1-4\rho^2\frac{\partial^2}{\partial\xi^2}\right)\left[M\frac{\partial^2\psi}{\partial\tau^2}+k\psi-(N-w\psi)\delta\left(\frac{\xi+1}{2}-\tau\right)\right]=0 \tag{2}$$

2.5 Boundary conditions

In this paper, the boundary conditions of Double Simply-supported and Clamped Simply-supported are considered. The equations related to the boundary conditions (3, 4, 5, and 6) are written based on the governing equation (1) for the dimensional case and the equations of the boundary conditions (7, 8, 9, and 10) are written based on the dimensionless governing equation (2).

The boundary conditions are as follows:

Boundary condition 1 (Double Simply-supported):

$$Y(0,t)=\frac{\partial^2 Y(x,t)}{\partial x^2}\Big|_{x=0}=0, \tag{3}$$

$$Y(L,t)=\frac{\partial^2 Y(x,t)}{\partial x^2}\Big|_{x=L}=0. \tag{4}$$

$$\psi(-1,\tau)=\frac{\partial^2\psi(\xi,\tau)}{\partial\xi^2}\Big|_{\xi=-1}=0, \tag{5}$$

$$\psi(1,\tau)=\frac{\partial^2\psi(\xi,\tau)}{\partial\xi^2}\Big|_{\xi=1}=0. \tag{6}$$

Boundary condition 2 (Double Simply-supported):

$$Y(0,t)=\frac{\partial Y(x,t)}{\partial x}\Big|_{x=0}=0, \tag{7}$$

$$Y(L,t)=\frac{\partial^2 Y(x,t)}{\partial x^2}\Big|_{x=L}=0, \tag{8}$$

$$\psi(-1,\tau)=\frac{\partial\psi(\xi,\tau)}{\partial\xi}\Big|_{\xi=-1}=0, \tag{9}$$

$$\psi(1,\tau) = \frac{\partial^2\psi(\xi,\tau)}{\partial\xi^2}\bigg|_{\xi\,=\,1} = 0. \qquad (10)$$

To solve the equations, Mathematica software is used. Mathematica is a powerful computational software. This software is a complete tool for performing mathematical calculations, data analysis, algorithm development, simulations and visualizations that allows creating complex codes and custom functions. This software has the ability to perform symbolic, numerical, matrix, functional, probabilistic and statistical calculations. You can use molecular dynamics equations, finite element method, vibration theory and by choosing the type of element, shape and size, materials and properties, boundary conditions and external forces, create the desired model and view the results numerically and graphically.

3. Discussion

To verify the accuracy of the solution method, the results have been compared with the exact solution. Also, the convergence of the solution has been investigated. In addition, by performing a case study, the dynamic behavior of CNT for different boundary conditions has been analyzed. Finally, the effect of nanoparticle velocity has been determined and the approximate critical velocities have been calculated. The codes are provided by MATHEMATICA 8. If the value of a geometric or physical parameter is not mentioned, the following properties are used for a single-walled nanotube and a C 60 as a fullerene.

$\rho = 0.1$ k=20 w=50 l=30nm $m_c=4.32\times10^{-15}$kg/m EI=7.12×10^{-25}Nm^2 m=1.196×10^{-24} kg v=50m/s g=9.81

In addition, the maximum degree of Legendre polynomials is kept constant: r = 8.

3.1 Convergence analysis

For this problem, convergence analysis is a difficult task. For this reason, we have used Mathematica software. The boundary conditions also affect the convergence. Each boundary condition should be considered separately. Figures (2 and 3) show the dimensionless deflection of CNT under the influence of nanoparticle in the Double Simply supported and mid - point of the Double Simply supported states, respectively. Also, figures (3 and 4) show the dimensionless deflection of CNT under the influence of nanoparticle in the Clamped Simply-supported and mid - point of Clamped Simply-supported states, respectively.

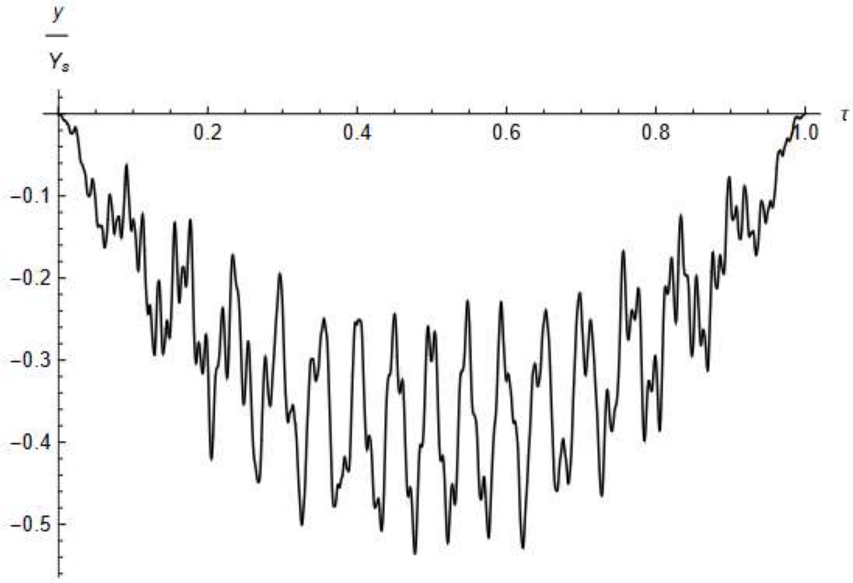

Fig.2. Vibration of the Double Simply supported CNT under moving Nano – particle

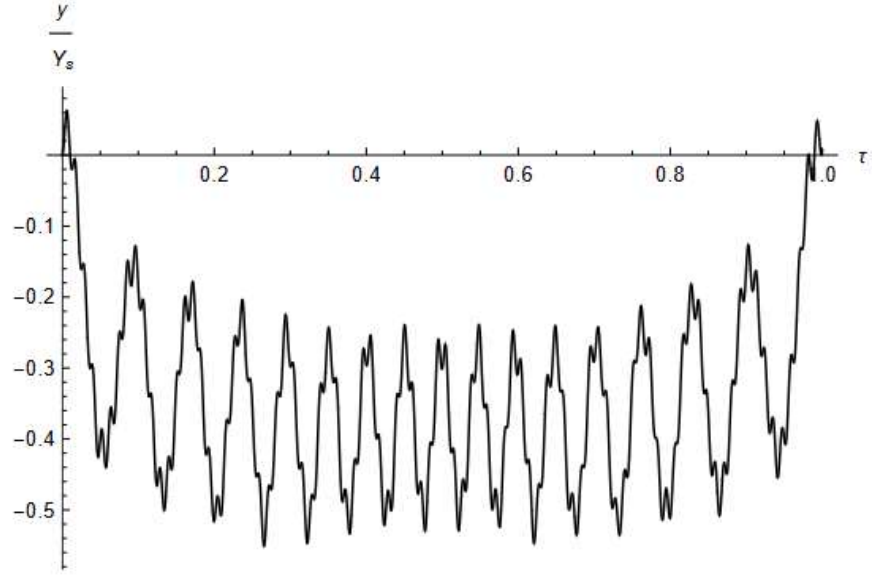

Fig.3. Vibration of the mid - point of the Double Simply supported CNT

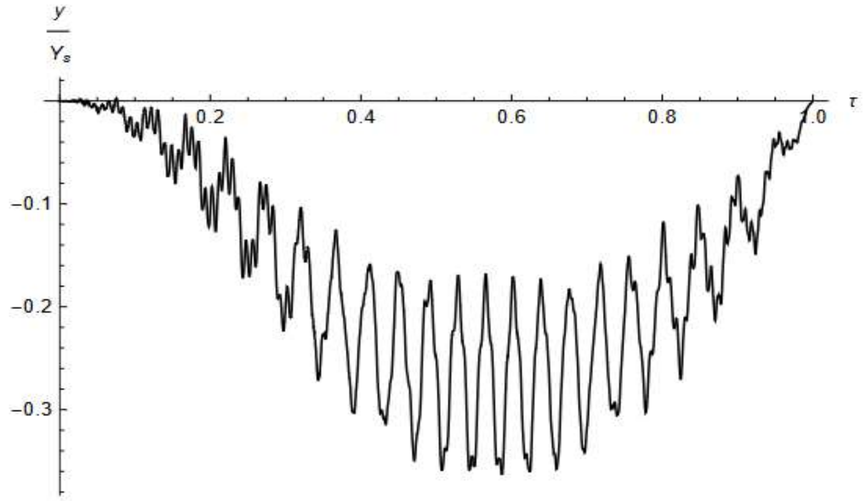

Fig.4. Vibration of the Clamped - Simply supported CNT under moving Nano – particle

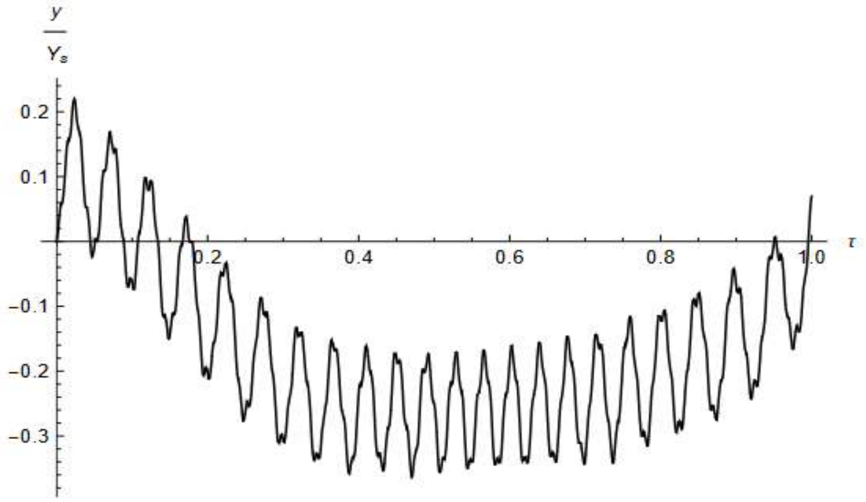

Fig5. Vibration of the mid - point of the Clamped - Simply supported CNT

4. Conclusion

In this paper, the interaction between a nanoparticle and a single-walled carbon nanotube using the nonlocal Euler-Bernoulli beam theory was investigated. In this study, it was assumed that CNT is subjected to different boundary conditions (Clamped Simply-supported, Double Simply-supported) and is on an elastic base and the van der Waals force is modeled by a confined spring. Also, a semi-analytical method based on Galerkin along with step-by-step DQ methods was used to solve the governing equation. The results showed that by increasing the foundation stiffness, the overall stiffness of the system increases and as a result, the dynamic displacement of CNT decreases. Finally, an empirical method was used to estimate the critical velocity and the results showed that CNT has the highest amplitude of vibration at the lowest critical velocity. In addition, it was concluded that the order of the first critical velocities for these boundary conditions is as follows:

It can be concluded that the use of carbon nanotubes in drug delivery for cancer patients can be effective. Because the results have shown that carbon nanotubes have the highest amplitude of vibration at the lowest critical speed, and this can mean that this feature can be useful in creating mechanical vibrations inside the body to stimulate cancer cells and increase their permeability for drugs.

Therefore, the use of carbon nanotubes in drug delivery for cancer patients can have significant improvements in the absorption and stabilization of drugs in the required location, reducing side effects and increasing therapeutic efficacy. However, to confirm these results and evaluate the performance of carbon nanotubes in drug delivery more accurately, more experiments and clinical studies are needed.

5. Suggestions and advantages

The combination of gold nanoparticles and carbon nanotubes in drug delivery can be very useful. By combining these two nanoparticles, the capabilities of each can be improved and cancer treatment can be enhanced. Carbon nanotubes are known as a nanoscale structure with unique properties in drug delivery and cancer detection. Also, gold nanoparticles are used as another nanoscale structure with prominent electronic and optical properties.

Ultimately, by combining carbon nanotubes and gold nanoparticles, good efficiency can be obtained from the properties of each of these nanomaterials in cancer detection and treatment. This combination can have a significant improvement in the permeability of cancer cells to anti-cancer drugs and also by creating mechanical vibrations in them, destroy cancer cells. Therefore, by combining carbon nanotubes with gold nanoparticles, the ability to deliver drugs more accurately and effectively to cancer cells increases. Carbon nanotubes can absorb drugs in themselves and use gold nanoparticles to deliver them to the desired areas in a targeted manner.

This method has advantages such as reducing side effects, increasing drug efficacy, reducing treatment costs and improving the quality of life of patients.

However, for practical use of this combination, more research and clinical trials are needed. This includes more studies on the effects of this combination in different conditions and on different types of cancers, evaluating the risks and safety of it, and determining the best conditions for using it for cancer treatment.

In general, the combination of carbon nanotubes and gold nanoparticles can be a new and reliable method in cancer detection and treatment. Although more research and clinical trials are needed, it is hopeful that this combination can be used as an effective treatment method in the fight against cancer in the near future.

To continue this research, it is suggested:

The effect of the combination of carbon nanotubes and gold nanoparticles on the vibrations of carbon nanotubes with different boundary conditions and in different environments should be studied.

The effect of the combination of carbon nanotubes and gold nanoparticles on the toxicity, biological and safety properties of carbon nanotubes should be evaluated.

The effect of the combination of carbon nanotubes and gold nanoparticles on different types of cancers and compare it with existing treatment methods should be investigated.

REFERENCES

[1] Article: "Carbon nanotubes as drug delivery vehicles" by K. Kam and T.H. Jessop. Published in 2005 in the journal "International Journal of Nanomedicine".

[2] Liu, Z., Sun, X., Huang, H., Gao, M., & Fan, K. (2020). Carbon nanotubes as nanodelivery systems for anticancer drug delivery. Expert Opinion on Drug Delivery, 17(3), 299-314.

[3] Liu, Z., Chen, K., Davis, C., Sherlock, S., Cao, Q., Chen, X., & Dai, H. (2008). Drug delivery with carbon nanotubes for in vivo cancer treatment. Cancer Research, 68(16), 6652-6660.

[4] Pantarotto, D., Singh, R., McCarthy, D., Erhardt, M., Briand, J. P., Prato, M., & Kostarelos, K. (2004). Functionalized carbon nanotubes for plasmid DNA gene delivery. Angewandte Chemie International Edition, 43(39), 5242-5246.

[5] Wang, S., Liu, X., Wang, Y., Zhang, Y., & Yu, L. (2019). Carbon nanotubes as a drug delivery system for anticancer therapies. Journal of Nanomaterials, 2019.

[6] Kam, N.W.S., O'Connell, M., Wisdom, J.A., and Dai, H. (2005). Carbon nanotubes as multifunctional biological transporters and near-infrared agents for selective cancer cell destruction. PNAS, 102(33), 11600-11605.

[7] Liu, Z., Chen, K., Davis, C., Sherlock, S., Cao, Q., Chen, X., & Dai, H. (2008). Drug delivery with carbon nanotubes for in vivo cancer treatment. Cancer research, 68(16), 6652-6660.

[8] Zhang, L., Xia, J., Zhao, Q., Liu, L., Zhang, Z., Zhang, Q., ... & Li Y. (2019). Carbon nanotube-mediated delivery of nucleic acids: Progress and perspectives. Nanomedicine, 14(3), 295-312.

[9] Liu, Z., Winters, M., Holodniy, M., & Dai, H. (2007). siRNA delivery into human T cells and primary cells with carbon-nanotube transporters. Angewandte Chemie International Edition, 46(12), 2023-2027.

[10] Liu, Z., Sun, X., Nakayama-Ratchford, N., Dai, H. (2007). Supramolecular chemistry on water-soluble carbon nanotubes for drug loading and delivery. ACS Nano, 1(1), 50-56.

[11] Liu, Z., Cai, W., He, L., Nakayama, N., Chen, K., Sun, X., ... & Chen, X. (2007). In vivo biodistribution and highly efficient tumour targeting of carbon nanotubes in mice. Nature nanotechnology, 2(1), 47-52.

[12] Cheng, Z., Liu, S., Shi, H., Jin, Y., Ji, J., & Li, C. (2012). Versatile carbonaceous nanospheres for biomedical applications. Chemical Communications, 48(83), 10277-10279.

[13] Bianco, A., Kostarelos, K., & Prato, M. (2005). Applications of carbon nanotubes in drug delivery. Current Opinion in Chemical Biology, 9(6), 674-679.

[14] Sun, X., Liu, Z., Welsher, K., Robinson, J. T., Goodwin, A., Zaric, S., & Dai, H. (2008). Nano-graphene oxide for cellular imaging and drug delivery. Nano research, 1(3), 203-212.

[15] Pantarotto, D., Briand, J. P., Prato, M., & Bianco, A. (2004). Translocation of bioactive peptides across cell membranes by carbon nanotubes. Chemical Communications, (1), 16-17.

[16] Liu, Z., Tabakman, S., Welsher, K., & Dai, H. (2009). Carbon nanotubes in biology and medicine: in vitro and in vivo detection, imaging and drug delivery. Nano research, 2(2), 85-120.

[17] Kam, N. W. S., & Dai, H. (2005). Carbon nanotubes as intracellular protein transporters: generality and biological functionality. Journal of the American Chemical Society, 127(16), 6021-6026.