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An Approach to Pancreatic Cancer Phototherapy Using CNTs and Carbon Dots

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Abstract
With a variety of available therapy options to alleviate cancer discomfort, all malignancies are not curable. To treat pancreatic cancer, a combination of radiation, chemotherapy, surgery, and light treatment is common. The potential of light therapy in pancreatic cancer therapy should be investigated. Tumor photon absorption enhancement is an important aspect of phototherapy. COMSOL is employed to look into how well single-walled and multi-walled carbon nanotubes (CNTs) absorb light photons in cancer tissue and how their temperature rises with the presence of the CNTs. The investigated parameters are nanotube length, diameter, simultaneous radiation of light photons in different directions, distances among CNTs, number of nanotube walls, and the carbon dots (CDs) crystal layer. The findings show that increasing the length and diameter with lightening in multiple directions, and the density of the nanotubes' volume all help improve the light photons' absorption. An increase in the distance between nanotubes significantly impacts the absorption enhancement of optical photons. Additionally, incorporating a crystal layer of CDs enhances the absorption, however, optimizing the thickness of the CDs is essential. Overall, the research findings show that the presence of CNTs in cancer tissue enhances their light absorption and increases the temperature of the cancer tissue.

Keywords: Photothermal Therapy, COMSOL, Cancer Therapeutics, Carbon Nanostructures of CNTs and Dots.

1. Introduction

One of the most important challenges facing mankind in terms of health is a group of diseases called "cancer". Cancer begins with the abnormal growth and division of body cells. Unfortunately, in some cancers, this abnormal growth of cells also spreads to other tissues [1,2]. There are different types of cancer. Unfortunately, it kills a large number of people every year. Intestinal cancer, liver cancer, and skin cancer are examples of cancers. The pancreas is a pear-shaped lesion 10 to 15 cm long that is located behind the stomach (between the stomach and the spine), and the end of the stomach extends to the spleen. The pancreas produces insulin and some hormones [3,4]. These hormones help the body consume and store energy from food. Also, this organ produces pancreatic juice, which contains enzymes that help digestion. This organ is anatomically divided into the head, trunk, and tail. The pancreas is the only endocrine and exocrine organ; that is, it releases some secretions into the blood. Some exocrine glands of this organ help digest and absorb food [5]. Typically, pancreatic cancer develops in the ducts responsible for directing the pancreatic fluids. When cancer metastasizes beyond the pancreas, it often infiltrates the lymph nodes, resulting in the spread of cancer cells to the surrounding organs, such as the liver and lungs. The worldwide rate of pancreatic cancer ranges from 5% to 8% [6,7]. Mortality from this type of cancer is also increasing. Since the diagnosis of this disease is in advanced stages, the death rate due to this cancer is high. Factors such as lifestyle, occupational exposure, and diet influence the development of cancer in the body. Diagnosis and treatment are two important steps to control this disease, which, with the advancement of technology, is trying to make the patient recover completely [8-10]. Time plays an important role in the process of disease control or treatment. The shorter the diagnosis time, the more the specialist can provide the best solution. Diagnosing pancreatic cancer typically involves evaluating personal and family medical histories as the initial step. Then, physical examinations are performed. Blood biochemistry tests, cancer biomarkers, and imaging tests such as computed tomography, magnetic resonance imaging, angiography, positron emission imaging, angiography, and endoscopy, are performed [11,12] as the process stages. The cutting-edge technology will significantly enhance the patient's full recovery, during the therapy. The classification, site, and extent of cancer advancement are crucial factors in selecting the appropriate treatment modality [13]. The treatment modalities include radiation, chemotherapy, surgery, hyperthermia, immunotherapy, and light therapy [14,15]. The study suggests using phototherapy as a therapeutic approach for pancreatic cancer. Nanotechnology has revolutionized cancer treatment by using nanostructures that can efficiently absorb and convert light into heat, enabling the application of photo-thermal therapy [16,17]. Utilizing photo-thermal therapy in conjunction with conventional cancer therapies would enhance therapeutic efficacy markedly. While it would mitigate the adverse effects associated with other approaches [18]. Recently, electromagnetic waves in the visible and infrared spectrum have been used for several forms of cancer treatment. An extensive study has been conducted in this sector up until the present day, based on this premise. Both normal and malignant cells are susceptible to heat [19,20]. Using lasers of varying intensities is one way to kill cancer cells. Raising the temperature kills cancer cells. Tumors are acidic and exposed to hypoxia, and cancer cells have a lower pH than healthy cells [21]. Consequently, it will be destroyed by a considerable rise in temperature. In most cases, malignant tumors are treated with high-power lasers. There are fewer adverse effects and a quicker recovery time associated with laser usage. Among these outside-the-body approaches to cancer treatment is photo-thermal therapy [22,23]. One potential use of nanoparticles in photothermal treatment is as an extrinsic absorption agent. Biosensors and medication release are only two examples of the various medicinal applications of carbon nanotubes in modern research [24]. The single-walled nanotubes are completely harmless when they harm bodily cells or set off the immune system. Research has also shown that targeted medication delivery and increased solubility are both enhanced by single-walled nanotubes [25,26]. The very high electrochemically active surface, high electrical conductivity, and good structural properties of single-walled and multi-walled carbon nanotubes make them a great choice for highly sensitive and non-invasive glucose sensors. The type and dimensions of nanoparticles are chosen, so they have the most absorption in the wavelength range of 700 to 2500 nm. This area is called tape therapy [27,28]. The middle area of the tape therapy is very suitable for working with lasers because the absorption of healthy tissue is minimal. While the absorption of nanotubes and nanoshells is very high. The effective factors in photo-thermal therapy with light lasers are the type and type of nanoconcentration and dimensions, the wavelength and intensity of laser light, and the duration of tissue exposure to radiation. Incorrect choices of intensity and duration of radiation hurt the treatment, so it is necessary to estimate the appropriate values and check the treatment's results through simulation [29,30]. In this research work, we will introduce and investigate the treatment of pancreatic cancer using phototherapy in the presence of carbon nanostructures using COMSOL software.

2. Materials and Methods

The first step in investigating cancer treatment using optical photons is to calculate the absorption coefficient of optical photons due to the application of an electric field caused by the radiation of electromagnetic waves. Analytical solutions of Maxwell's equations can be obtained using the Mie theory for spherical particles. However, numerical approaches are required to obtain the solution to Maxwell's equations for non-spherical geometries. In this study, we used the radio frequency module of COMSOL software to solve Maxwell's equations. It was also implemented from a fully matched layer to shorten the computational domain [31,35]. In addition to the absorption property of the absorption layer and to reduce the effect of discretization, a scattering boundary condition was assigned to the outermost surface, which means that the waves that reach the outer boundary of the computational domain do not return to the desired domain. The amount of scattered and absorbed light was determined using cross-section calculations. The particle absorption cross-section, σ_{abs}, can be calculated from the Poynting theorem as follows [34,33]:

$$\boldsymbol{\sigma}_{\boldsymbol{abs}} = \frac{\boldsymbol{W_{abs}}}{\boldsymbol{S_{in}}} \tag{1}$$

The Poynting vector, S_{in}, represents an electromagnetic field's directional energy flux (energy transfer per unit area, per unit time) or power flow. The SI unit of the Poynting vector is watt per square meter. In equation 1, the absorption coefficient of light photons by carbon nanotubes is obtained by dividing the absorbed power per unit area of carbon nanotubes by the size of the pointing vector. Where S_{in} is the size of the Poynting vector and the absorbed power by the nanoparticle is [34]:

$$W_{abs} = \iiint_V Q_h dV \tag{2}$$

In equation 2, the Q_h is the total power loss density of the calculated electromagnetic fields. Therefore, the total absorbed power is obtained by dividing by the volume of nanoparticles. Also, to calculate the absorbed power by carbon nanotubes (CNT), the volume integral can be taken from the heat loss density over the nanotube volume. Calculating the absorbed power of nanoparticles as a heat source: The absorption properties of nanoparticles play an important role in photo-thermal heating. At the LSPR wavelength, the absorbed light and the photo-thermal heating effect are maximized. To calculate the photo-thermal heating produced by a spherical nanoparticle, the following equation has been used [34]:

$$Q_s = \frac{I_S \sigma_{abs}}{V} \tag{3}$$

In equation 3, Q_s represents the power density absorbed per unit volume, ignoring any loss, which refers to the heating caused by the absorption of optical photons by carbon nanotubes within the tissue ($Q_h \approx Q_s$). Here, σ_{abs} is the absorption coefficient of optical photons, I_s is the flux of incoming photons and V is the nanotubes's volume [34]. In this research, the effect of the following parameters on the absorption of thermal photons for the treatment of pancreatic cancer in the presence of carbon nanotubes has been investigated:

1- Optical photon absorption cross-section in the presence of single-walled and multi-walled carbon nanotubes (SWCNT)

2- The effect of the height of single-walled and multi-walled nanotubes (MWCNT) on the absorption of optical photons

3- The effect of the diameter of SWCNT

4- Effect of volumetric knowledge of SWCNT on the absorption of optical photons

5- The effect of the presence of CDs on the absorption coefficient of optical photons in SWCNT

6- The effect of layer thickness on absorption coefficient.

3. Results and Discussion

In this research, COMSOL software was used to investigate the effect of carbon nanotubes in absorbing light photons and generating heat in pancreatic cancer cells. For this purpose, electromagnetic wave modules have been used in the field of frequency and heat transfer in a stable state. Therefore, the modeling of this project has been done in two phases:

1- Calculation of absorption coefficient of optical photons by carbon nanotubes in different conditions

2- Calculation of heat generated in cancer tissue by carbon nanotubes in different conditions.

3.1. The cross-sectional area of light photon absorption by single-walled

In the first step, a SWCNT inside a sphere made of water is generally considered. We consider the homogeneous tissue of the tumor made of water and examine the absorption of light photons and the amount of heat produced inside this sphere in the presence of carbon nanotubes. For this purpose, a sphere with a diameter of 200 nm made of water is considered. Two concentric cylinders were with different diameters to introduce the carbon nanotube. For optimization of the diameter of CNT, we define CNT with different diameters and then calculate the absorption coefficient of CNT in the frequency range of the photon source. We used the electromagnetic module of COMSOL software to calculate the absorption coefficient for CNT. The schema of the model defined in COMSOL is shown in Figure 1.

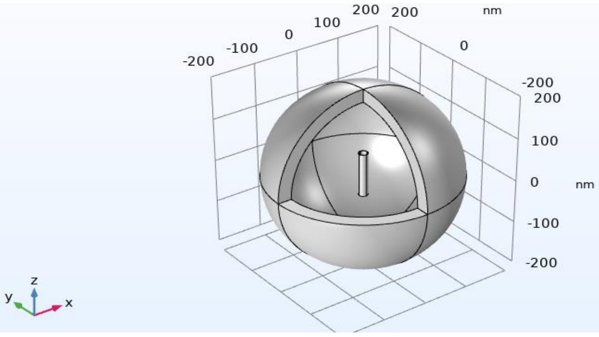

Fig.1. The schematic of SWCNT and media in COMSOL

The intensity of the electrical field created in three-dimensional form as well as the cross-sectional view of the electric field created in the x-y plane in the presence of SWCNT is shown in Figure 2. As can be seen in Figure 2, the intensity of the electric field on the carbon nanotube is higher than in other places. Also, the σabs of SWCNT are shown in Table 1. In the simulation shown in Figure 2, the dimensions of the carbon nanotube are specified as follows: the inner cylinder height is 10 nanometers, and the nanotube diameter is 200 nanometers.

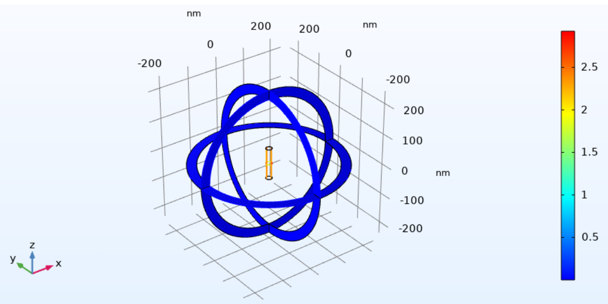

Fig.2. The electrical field in the presence of SWCNT

Table 1. σ_{abs} of Light on SWCNT

λ(nm)	σ_{abs}(nm^2)
700	139
750	517
800	85

As we know, the longer the nanotube the more pronounced its properties become, the effect of nanotube length on the absorption coefficient is investigated. The nanotube length impact on the absorption coefficient of optical photons for lengths of 50, 100, 150, and 200 nm was investigated.

Table 2 shows the photon absorption coefficient for SWCNTs with different lengths and Figure 3 illustrates the absorption coefficient of SWCNTs for varying diameters.

Table 2. Optical absorption cross-section, σ_{abs} (nm^2), for SWCNT with different lengths

λ(nm)	σ_{abs} (nm^2)			
	L=5nm	L=100nm	L=150nm	L=200nm
700	70	139	280	277
750	254	517	780	1043
800	43	85	126	1068

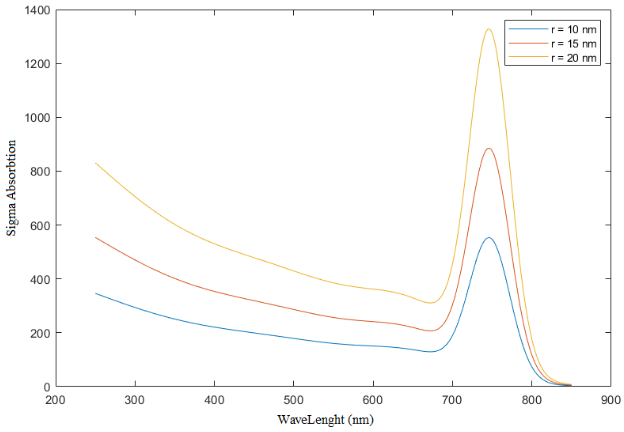

Fig.3. σ_{abs} of SWCNT with different diameter

Investigating the effect of nanotube diameter on the absorption coefficient, in this part, the effect of increasing the diameter of single-walled carbon nanotubes on the absorption coefficient of optical photons has been investigated. Therefore, the absorption coefficient has been calculated for SWCNT with diameters of 5, 10, 15, and 20 nm. Table 3 shows the absorption coefficient of optical photons for single-walled carbon nanotubes with varying diameters.

Table 3. Optical photon absorption coefficient for nanotubes with different diameters

λ(nm)	σ_{abs} (nm^2) in different diameters (nm) of SWCNT			
	d=5nm	d=100nm	d=150nm	d=200nm
700	76	139	203	267
750	218	517	723	912
800	29	85	147	210

3.2. Investigating the effect of increasing the distance of carbon nanotubes from each other

In this part, the effect of increasing the distance of single-walled carbon nanotubes from each other on the absorption coefficient of optical photons has been investigated. Therefore, the absorption coefficient has been calculated for the center-to-center distance of three nanotubes with a diameter of 10 and a height of 100 nm with distances of 20 nm, 50 nm, and 80 nm. Table 4 demonstrates the effect of increasing the center-to-center distance between single-walled carbon nanotubes on the absorption coefficient of optical photons.

Table 4. Optical photon absorption coefficient for nanotubes with different center-to-center distance

λ(nm)	σ_{abs} (nm^2) with different distances (nm)		
	d =5nm	d=150nm	d=200nm
700	422	419	419
750	1399	1534	1539
800	312	263	258

Table 5. Optical photon absorption is the coefficient for different numbers of nanotubes in constant volume

λ(nm)	σ_{abs} (nm^2) with different numbers of CNT		
	1	3	9
700	139	422	1100
750	517	1399	4450
800	85	312	750

Table 6. Optical photon absorption coefficient for multi-walled nanotubes

λ(nm)	σ_{abs} (nm^2) with different numbers of Layers		
	1	2	3
700	139	231	568
750	517	1047	1358
800	85	143	193

3.3. Investigating the effect of increasing the volumetric density of SWCNT

Increasing the volume density of carbon nanotubes is one of the main parameters of its absorption coefficient. Therefore, the absorption coefficient of optical photons by one, three, and nine carbon nanotubes with a diameter of 10 nm, a height of 100 nm, and a center-to-center distance of 20 nm has been investigated. Table 5 illustrates the absorption coefficient of optical photons by different numbers of single-walled carbon nanotubes within a constant volume.

3.4. Investigating the effect of the distance of SWCNT from each other on heat distribution

One of the important factors in the absorption of light photons by the tissue is the uniform distribution of heat in the tissue so that the entire tissue can be treated uniformly. In this part, the effect of the distance of nanotubes from each other on the uniformity of heat distribution in the tissue has been investigated. Figure 4 shows the heat distribution in the tissue with varying center-to-center distances between single-walled carbon nanotubes, illustrating the uniformity of heat spread.

3.5. Investigating the effect of MWCNT on the absorption coefficient

Multi-walled carbon nanotubes are created in the form of interlaced hollow cylinders. In this part, the effect of single-walled nanotubes with a diameter of 10 and a thickness of 0.1 nm, double-walled with a diameter of 10 and a thickness of each layer of 0.1 nm, and three-walled with a diameter of 10 and a thickness of each layer of 0.1 nm, on the absorption coefficients were investigated. Table 6 presents the absorption coefficient of optical photons for multi-walled carbon nanotubes with one, two, and three layers.

3.6. Investigating the effect of the incoming photon flux on the generation of heat

One of the influencing parameters on the heat created in the tissue is the flux of incoming photons. Therefore, in this part, the amount of heat generated in different fluxes of 10^{-9}, 10^{-8}, 10^{-7}, and 10^{-6} photons per unit area for a single-walled nanotube with a diameter of 10 and a height of 100 nm has been investigated. Figure 5 shows the effect of varying photon flux on heat generation in the tissue for single-walled nanotubes, highlighting the relationship between photon flux and heat production.

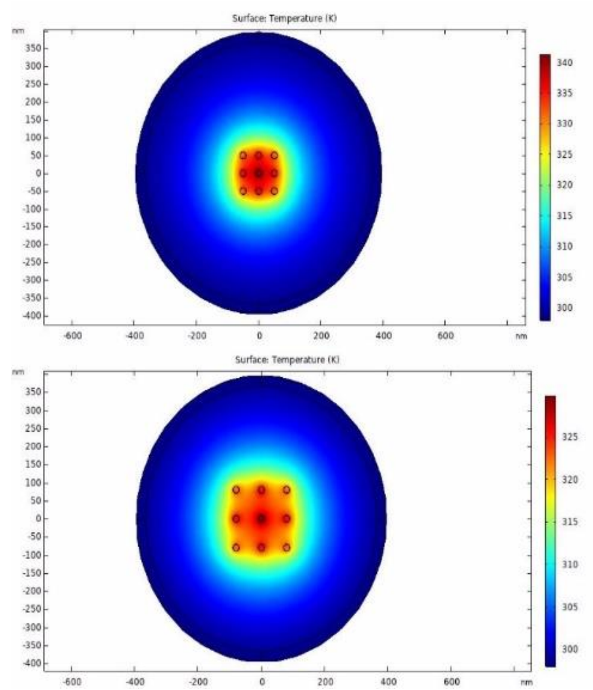

Fig.4. The heat distribution in the presence of SWCNT with the different center-to-center distances: a) 50 nm, b) 80 nm.

3.7. Investigating the effect of CDs on the absorption coefficient of SWCNT

Different materials can be added to carbon nanotubes to increase the absorption of light photons. For this purpose, amino acid compounds can be added that can penetrate the body tissues and have a suitable reactivity with carbon nanotubes. One of the materials that can be used to increase the absorption coefficient of carbon nanotubes are CDs crystal. CDs are semiconductors with a band gap of 2.42 eV and a maximum absorption peak at a wavelength of 514 nm, which indicates that CDs can absorb visible light and UV light at wavelengths longer than 514 nm. This makes CDs an efficient photocatalyst. In addition, the band gap position of CDs is suitable for many photocatalytic reactions such as water splitting and CO_2 reduction. CDs have been widely investigated as a photo-catalyst. Notably, the position of the conduction band edge of CDs is lower than that of other common semiconductors such as TiO_2, ZnO, and $SrTiO_3$. This means that in the photocatalytic reaction, CDs photoelectrons have strong reducing power. However, CDs materials are prone to corrosion by light. This limits the number of CDs photo-catalysts that can be recycled. To solve this fundamental problem, researchers have proposed measures to improve the CDs photo-catalyst, which uses the ratio The most common method of preparing CDs composite materials is using different materials or ion doping methods. The CDs photo-catalyst increases the absorption at long wavelengths by using the composite, thus achieving higher photo-catalysis and recovery capability. Poly-amino-amides are used to add this crystal to carbon nanotubes. The effect of the layer of CDs with different thicknesses on the absorption coefficient of light photons and the heat generated by single-walled carbon nanotubes with a diameter of 10 and a height of 100 nm was investigated. Table 7 details the absorption coefficient of optical photons for single-walled carbon nanotubes with varying thicknesses of layers of CDs.

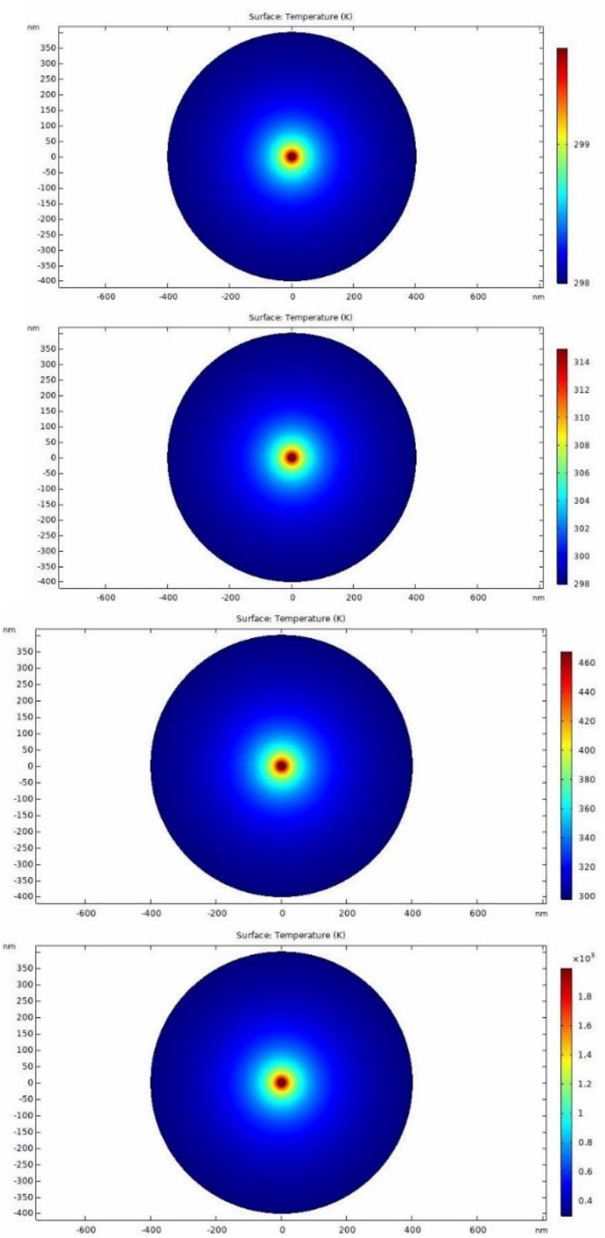

Fig.5. The effect of photon flux on production heat: a) 10^{-9}, b) 10^{-8}, c) 10^{-7}, d) 10^{-6} photons per unit area

Table 7. Absorption coefficient of optical photons for SWCNT with CDs of different thicknesses

λ(nm)	σ_{abs} (nm^2) with CDs layer		
	Single CNT	CNT + 1 nm CDs	CNT + 2 nm CDs
700	139	519	296
750	517	900	700
800	85	501	309

4. Conclusion

Pancreatic cancer remains a formidable challenge due to its late diagnosis and the invasiveness or collateral damage associated with traditional treatments like surgery, chemotherapy, and radiation therapy. Phototherapy, utilizing infrared waves, presents a promising non-invasive alternative, particularly when enhanced by the use of carbon nanotubes (CNTs). This study provides a comprehensive examination of the parameters affecting the absorption coefficient of optical photons by single-walled (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) and their implications for photothermal cancer treatments. The research, executed through meticulous simulations using COMSOL software, reveals that increasing the height and diameter of CNTs significantly boosts their absorption coefficient, thereby enhancing heat generation in cancerous tissues. It was also found that multi-directional irradiation further amplifies this effect compared to unidirectional approaches. An essential insight from the study is that while varying the center-to-center distance between nanotubes at a constant volume density does not change the absorption coefficient, it does impact the uniformity of heat distribution, which is critical for effective treatment. Moreover, increasing the volumetric density of CNTs uniformly enhances the absorption coefficient and tissue temperature, confirming the efficacy of densely packed nanotube configurations. The comparative analysis indicates that MWCNTs have superior photon absorption capabilities over SWCNTs, leading to more effective cancer cell destruction via hyperthermia. Furthermore, the integration of Carbon dots (CDs) crystals into the nanotube structure shows significant improvement in absorption, with optimal layer thickness being crucial for maximizing efficacy without diminishing returns. The implications of these findings are profound for the advancement of photothermal cancer therapies. This research lays a robust foundation for developing more precise and effective treatment modalities by optimizing nanotube dimensions, irradiation methods, and composite structures. The versatility of CNTs demonstrated through their enhanced absorption properties and potential for customization, positions them as pivotal components in the future of nanotechnology applications in medicine.

5. Suggestions for Future Work

Future research should focus on in vivo studies to validate the simulation findings and investigate the long-term effects and safety of CNT-based photothermal treatments. Moreover, the synergistic effects of combining CNTs with other therapeutic agents investigation could significantly enhance the overall efficacy of cancer treatments. Exploring the potential of CNTs in various types of cancer such as breast cancer and medical applications like drug delivery systems could significantly broaden their utility and impact the field of nanomedicine.

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