#### Research Article

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# Arrangement structure of carbon nanofiber with excellent spectral radiation characteristics

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**Abstract:** To explore the spectral radiation characteristics of carbon nanofibers, a finite-difference time-domain method has been applied to study and calculate the scattering/ absorption factors of carbon nanofibers with various arrangements, while the filler contents are 61.15%, 53.81%, 48.92%, 44.03% and 39.13% in the spectrum band of 2.5-15 µm. The effects of the nanofiber content, 2D/3D random arrangement and nanofiber radius on scattering/ absorption characteristics have been analyzed. The analytical results show that the spectral radiation characteristics of carbon nanofibers have been significantly increased with an increase in the filler content. When the nanofiber content reduced to 48.92%, the random arrangement structure of carbon nanofiber plays an essential role in determining the spectral radiation characteristics. Analytical results prove that the prediction accuracy has been significantly improved by 30.12% by sing the 3D random arrangement model than by using the 2D uniform arrangement model. This study proposed a 3D model to predict the spectral radiation characteristics of carbon nanofibers and their aggregates in engineering nanocomposites.

**Keywords:** spectral radiation characteristics, carbon nanofiber, time domain method, random arrangement

### 1 Introduction

Carbon nanofiber has good heat resistance and corrosion resistance [1–4] and act as a reinforcement for various

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types of matrix materials in the form of nanocomposites [5–8]. Carbon nanofiber nanocomposites have good thermal insulation properties, and hence they are applied in some high-temperature protection fields, i.e., C/C nanocomposites in thermal protection materials for the high-speed aircraft [9,10]. Carbon nanofiber nanocomposites can be fabricated by weaving techniques to achieve the 3D design of various arrangements in the matrix [11]. A study on the spectral radiation characteristics of carbon nanofibers with different arrangements is of great significance for the nanocomposites at high temperatures, resulting in a high random distribution of nanofibers. Therefore, it is necessary to investigate the spectral radiation characteristics of carbon nanofibers with random distributions and to provide a theoretical approach to explore the working mechanism and constitutive relationship.

Currently, a large number of studies have been conducted to study the radiation characteristics of carbon nanofiber nanocomposites [12-15]. Many previous studies aim on experimental measurements of the emissivity or absorption rate of nanocomposites, which is incorporated from various arrangements of carbon nanofibers [16-18]. Balat-Pichelin et al. [19,20] prepared several types of 2.5D woven composites and measured the absorptivity and emissivity of carbon nanofibers at the same temperature to investigate the radiation characteristics of carbon nanofibers with various arrangement structures. Wang et al. [21-23] analyzed the effects of environmental factors and material structure on the thermal radiation characteristics of C/SiC composites. Lee [24] proposed a theoretical Mie solution model by means of the long cylindrical model. Lee [25,26] formulated a calculation approach to describe the thermal properties of closely arranged wireless parallel cylinders fibrous structures. Briana and Hyers [27] proposed a Monte Carlo formulation to predict the effect of alignment arrangement on the spectral absorbance and reflectance of carbon nanofibers. These theoretical 2D approaches are limited to study the radiation characteristics of carbon nanofibers with uniform distributions in the nanocomposite. However, it had been

found that the distribution state of the carbon nanofiber is random in the experiments [28,29]. Therefore, it is necessary to propose a work to study the effect of random arrangement of carbon nanofibers on radiation characteristics of nanocomposites. Also, more efforts have been taken in the previous studies to study the arrangement of carbon nanofibers uniform nanocomposites.

In this study, the finite-difference time-domain (FDTD) method was used to study the radiation characteristics of carbon nanofibers with various arrangements. Constitutive relationships among the nanofiber content, uniform arrangement and random arrangement parameters with scattering and absorption factors had been developed. Furthermore, the effects of the nanofiber content and the random arrangement on the spectral radiation characteristics of carbon nanofibers were studied. Meanwhile, the deviations of the scattering and absorption values under the uniform and random arrangement of carbon nanofibers were then compared. Furthermore, the spectral radiation characteristics of carbon nanofibers with different contents and their relative deviations were analyzed in the 2D and 3D random arrangement structures. The effects of nanofiber radius and random arrangement structure on the spectral radiation characteristics were theoretically analyzed and discussed.

### 2 Methodology

### 2.1 Theoretical formulation

The internal structure of the carbon nanofiber is complex, whereas the cross section of carbon nanofiber can be regarded as a circular based on the observation of electron micrographs [30]. In the simulation, the parallel light in the spectrum band of 2.5-15 µm has been used as the light source. The carbon nanofiber bundles are ruled by the multiple long cylindrical array models. The uniform radius of individual carbon nanofiber is 6 µm as shown in Figure 1(a) and (b), while the nonuniform radius of carbon nanofiber is ranged from 1 to 7 µm, as shown in Figure 1(c). The longitudinal direction of carbon nanofiber is parallel to the Z-axis. However, the carbon nanofibers are mixed with each other in a 3D random arrangement as shown in Figure 1(d). The complex refractive index of the carbon nanofiber is

similar to that of the graphite in the spectrum band of 2.5-15 um [31].

The FDTD model is governed by the following Maxwell equations [32,33]:

$$\begin{cases}
\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \\
\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} - \mathbf{J}_{m}
\end{cases} \tag{1}$$

where *E* is the electric field strength, *D* is the electric flux density, H is the magnetic field strength, B is the magnetic flux density, J is the current density and  $J_m$  is the magnetic flux density. In a Cartesian coordinate system, where electromagnetic waves propagate along the *x* direction, the Maxwell equation is then rewritten as follows [32,33]:

$$\begin{cases} -\frac{\partial H_z}{\partial x} = \varepsilon \frac{\partial E_y}{\partial t} + \sigma E_y \\ \frac{\partial E_y}{\partial x} = -\mu \frac{\partial H_z}{\partial t} + \sigma_{\rm m} H_z \end{cases}$$
 (2)

where  $\varepsilon$  is the dielectric constant of medium,  $\sigma$  is the electrical conductivity,  $\mu$  is the magnetic permeability and  $\sigma_{\rm m}$  is the magnetic permeability. x, y and z represent the x-axis, y-axis and z-axis directions, respectively. By using the FDTD method to discretize equation (2), the electric field and magnetic field components can be obtained as follows [32,33]:

$$E_x^{n+1}(k) = CA(m) \cdot E_x^n(k) - CB(m) \cdot \frac{H_y^{n+1/2} \left(k + \frac{1}{2}\right) - H_y^{n+1/2} \left(k - \frac{1}{2}\right)}{\Delta z}$$
(3)

$$H_{y}^{n+1/2}\left(k + \frac{1}{2}\right) = CP(m) \cdot H_{y}^{n-1/2}\left(k + \frac{1}{2}\right) - CQ(m) \cdot \frac{E_{x}^{n}(k+1) - E_{x}^{n}(k)}{\Delta z}$$
(4)

where  $\Delta z$  represents the size of the z-direction grid, k represents the kth grid in the z direction and m is the expression discrete from the node. Here, m = k, while the CA(m), CB(m), CP(m) and CQ(m) can be found in the previous studies [32,33]. To calculate the incident of the Poynting vector and average radiation intensity at the node, the component values of electric and magnetic fields are, respectively, expressed as follows [34]:

$$\mathbf{S}_{\text{inc}} = \text{Re}(\mathbf{E}_{\text{inc}}) \times \text{Re}(\mathbf{H}_{\text{inc}}) \tag{5}$$

$$I = \left| \frac{1}{T} \int_{0}^{T} \mathbf{S}(t) dt \right|$$
 (6)

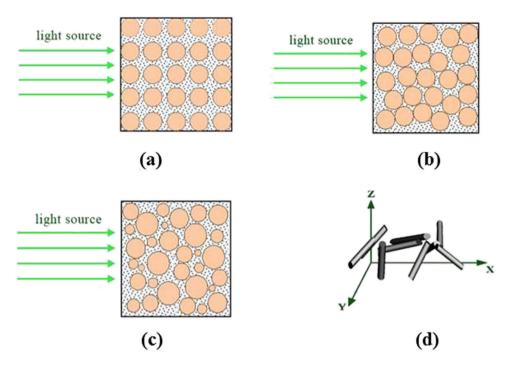


Figure 1: Illustration of the arrangement of carbon nanofibers in nanocomposite: (a) uniform arrangement of carbon nanofibers with radius of 6  $\mu$ m, (b) random arrangement of carbon nanofibers with radius of 6  $\mu$ m, (c) random arrangement of carbon nanofibers of with a radius range from 1 to 7  $\mu$ m and (d) 3D random arrangement of carbon nanofibers.

The cross-sectional scattering and absorption parameters are defined as follows:

$$C_{\text{scat}} = \frac{P_{\text{scat}}}{I_{\text{inc}}} \tag{7}$$

$$C_{\rm abs} = \frac{P_{\rm abs}}{I_{\rm inc}} \tag{8}$$

where  $P_{\rm scat}$  and  $P_{\rm abs}$  are the total scattered and absorbed powers, respectively. Both of these powers can be obtained using the power monitors in the scattering field region and the full field region with the aid of FDTD software. The scattering and absorption factors are expressed as follows:

$$Q_{\text{scat}} = \frac{C_{\text{scat}}}{A} \tag{9}$$

$$Q_{\rm abs} = \frac{C_{\rm abs}}{A} \tag{10}$$

where A is the sectional area of the cylinder carbon nanofiber in parallel to the light and along the x-axis.

Perfectly matched layer (PML) is a common method for absorption boundary by means of absorbing electromagnetic waves emitted from scatters or radiation sources in the calculation area. Since the wave impedance of PML exactly matches that of the simulation area, the dielectric impedance can be obtained [35]:

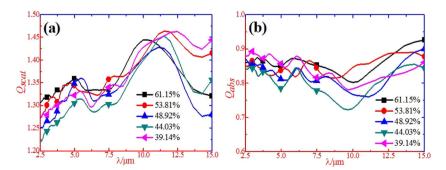


Figure 2: Analytical results of (a) scattering factor and (b) absorption factor with respect to various nanofiber contents of 61.15%, 53.81%, 48.92%, 44.03% and 39.14%.

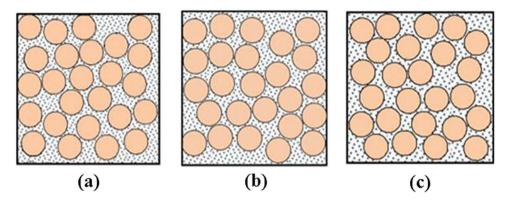


Figure 3: Random arrangement of 25 carbon nanofibers with a uniform radius. (a) case 1; (b) case 2; (c) case 3.

$$\frac{\sigma}{\varepsilon_0} = \frac{\sigma_m}{\mu_0} \tag{11}$$

The components of the electric and magnetic fields are [30,31] as follows:

$$E = E_0 \exp \left[ jw \left( t - \frac{x \cos \varphi + y \sin \varphi}{cG} \right) \right]$$

$$\cdot \exp \left( -\frac{\sigma_x \cos \varphi}{\varepsilon_0 cG} x \right) \cdot \exp \left( -\frac{\sigma_y \sin \varphi}{\varepsilon_0 cG} y \right)$$
(12)

$$H = H_0 \exp \left[ jw \left( t - \frac{x \cos \varphi + y \sin \varphi}{cG} \right) \right]$$

$$\cdot \exp \left( -\frac{\sigma_x \cos \varphi}{\varepsilon_0 cG} x \right) \cdot \exp \left( -\frac{\sigma_y \sin \varphi}{\varepsilon_0 cG} y \right)$$
(13)

where G is a given parameter [32,33], c represents the speed of light and  $\varphi$  is the angle between the field component and the coordinate system.

### 3 Results and discussion

### 3.1 Effect of nanofiber content on spectral radiation characteristics

To verify the accuracy of the FDTD model, analytical results of the radiation characteristics of carbon nanofibers have been presented in comparison with that of the Mie model [36]. The values of the complex refractive index of the carbon nanofiber are given constants [31].

For simulation of the 2D random arrangement of carbon nanofibers with nonuniform radius, the carbon nanofibers were randomly arranged in the dimensions of  $34 \, \mu m \times 34 \, \mu m$ . When the number of carbon nanofibers is

decreased from N = 25, N = 22, N = 20, N = 18 to N = 16, the nanofiber content is decreased from 61.15%, 53.81%, 48.92%, 44.03% to 39.14%. Figure 2 plots the effect of the nanofiber content on the scattering and absorption factors.

It is revealed that both the scattering and absorption factors are increased with an increase in the nanofiber content. In comparison with that of the nanocomposite incorporated, i.e., 39.14% carbon nanofiber, the relative deviation of the scattering factor decreased from 8.59%, 2.61%, 11.35% to 7.13% when the nanofiber content increased from 44.03%, 48.92%, 53.81% to 61.15%, whereas the relative deviation of the absorption factor decreased from 9.41%, 8.33%, 5.71% to 9%. In the entire spectrum band of  $2.-15\,\mu\text{m}$ , the average values of relative deviation of scattering factors are 2.36%, 1.23%, 1.74% and 2.61%, whereas that of the absorption factor are 2.36%, 3.98%, 3.45% and 5.47%.

These analytical results reveal that the relative deviations of both scattering and absorption factors increased with an increase in the nanofiber content. The influence of the nanofiber content on the absorption factor is greater than that of the scattering factor. The average relative deviation of the scattering and absorption factors are 5.47% and 2.61%, respectively, when the nanocomposites incorporated are of 39.14% and 61.15% carbon nanofiber. The higher nanofiber content results in higher spectral radiation characteristics of nanocomposite because the dense carbon nanofibers enhance the scattering and absorption of the light. These dense carbon nanofibers can significantly improve their interactive reactions and then improve the multiple scattering among carbon nanofibers. Therefore, the scattering factor of nanocomposite with the high nanofiber content is higher than that with the low nanofiber content.

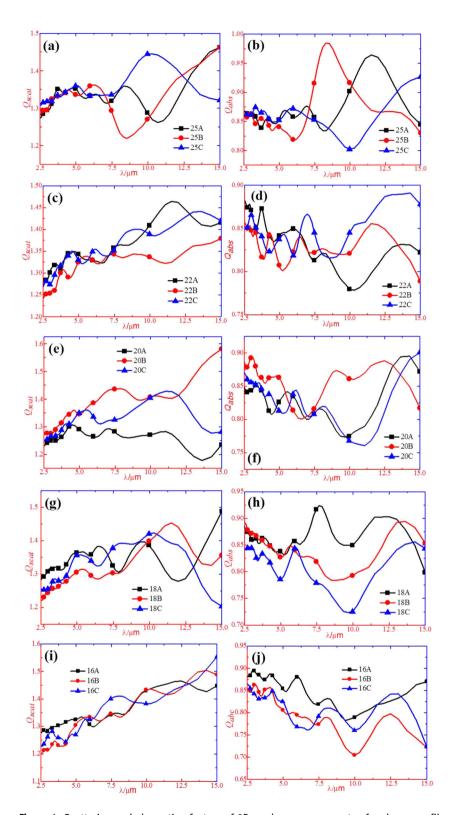
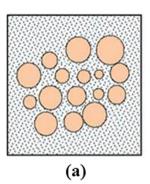
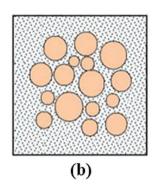


Figure 4: Scattering and absorption factors of 2D random arrangements of carbon nanofiber with various numbers: (a) 25, (b) 25, (c) 22, (d) 22, (e) 20, (f) 20, (g) 18, (h) 18, (i) 16 and (j) 16.





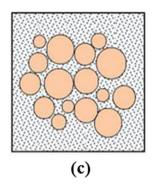


Figure 5: Random arrangements of carbon nanofibers with a content of 39.13% in nanocomposites. (a) case 1; (b) case 2; (c) case 3.

## 3.2 Analysis of spectral radiation characteristics of carbon nanofiber with random arrangement

As illustrated in Figure 3, there are three types of arrangements of carbon nanofibers. Figure 4 plots the analytical results of scattering and absorption factors with respect to the various numbers of carbon nanofibers, i.e., 25, 22, 20, 18 and 16. Based on the formula of relative mean deviation Rd =  $\left| \begin{array}{c|c} \frac{\mid X_1-\overline{X}\mid +\mid X_2-\overline{X}\mid +\mid X_3-\overline{X}\mid}{3\overline{X}} \end{array} \right| \times 100\%, \text{ where }$  $X_1$ ,  $X_2$  and  $X_3$  are the average sample values of A, B and C arrangement types, respectively, and  $\overline{X}$  is the average value of  $X_1$ ,  $X_2$ ,  $X_3$ ). Simulation results show that the relative mean deviations of scattering factors are 1.26%, 1.20%, 2.48%, 1.94% and 1.73% with a decrease in the nanofiber number from 25, 22, 20, 18 to 16. While that of the relative mean deviations of absorption factors are 1.72%, 1.47%, 4.14%, 2.43% and 2.25%. These analytical results show that the arrangement of the carbon nanofiber plays a more significant effect on the absorption factor than the scattering factor. However, the random arrangement has little effect on the spectral radiation characteristics of carbon nanofibers, whereas the relative mean deviations of the absorption factors are 1.67%, 1.27%, 1.11%, 0.91% and 0.62% in the shorter wavelengths from 2.5 to 7.5 µm. Meanwhile, relative mean deviations of the absorption factors gradually increased from 1.96%, 3.29%, 2.19%, 1.49% to 3.88% with an increase in the wavelengths from 7.5 to 15 µm.

The structure of carbon nanofibers is diverse although they have the same content and equal radius. When light waves are incident on the columnar carbon nanofibers with random arrangement, there are multiple scattering and coherent scattering among carbon nanofibers, resulting in a relative deviation in scattering and absorption property owing to the different arrangement structure. However, when the content and the diameter are confirmed, the effect of random arrangement of

carbon nanofibers on scattering factor is less. It is found that the deviations are less than 2% and 4% at the wavelengths of  $2.5-7.5\,\mu m$  and  $7.5-15\,\mu m$ , respectively.

## 3.3 Spectral radiation characteristics of carbon nanofiber with uniform/random arrangements

There are three types of arrangements of 16 carbon nanofibers with a radius ranging from 1 to  $7\,\mu m$ , as illustrated in Figure 5. Figure 6 plots the analytical results of scattering and absorption factors with respect to the various carbon contents of 61.15%, 53.81%, 48.92%, 44.03% and 39.13%. Analytical results show that the relative mean deviations of scattering factors are 1.89%, 1.31%, 1.96%, 1.57% and 1.46% with a decrease in the content from 61.15% to 39.13%, whereas the relative mean deviations of the absorption factors are 1.79%, 1.83%, 2.21%, 1.99% and 2.02%. These analytical results present that the nonequal radius plays a significant effect on the absorption factor compared to that on the scattering factor for the carbon nanofibers with random arrangements.

There are three types of arrangements of 16 carbon nanofibers with the radius ranging from 1 to 7  $\mu$ m. The random arrangement has little effect on the spectral radiation characteristics of carbon nanofibers, whereas the relative mean deviations of the absorption factors are 1.25%, 1.11%, 1.27%, 0.93% and 0.90% in the short wavelengths from 2.5 to 7.5  $\mu$ m. Meanwhile, the relative mean deviations of the absorption factors gradually increased from 1.89%, 2.31%, 3.08%, 3.44%, to 1.51% with an increase in the wavelength from 7.5 to 15  $\mu$ m. During the light wave being incident on the carbon nanofibers with nonequal radius, the multiple scattering

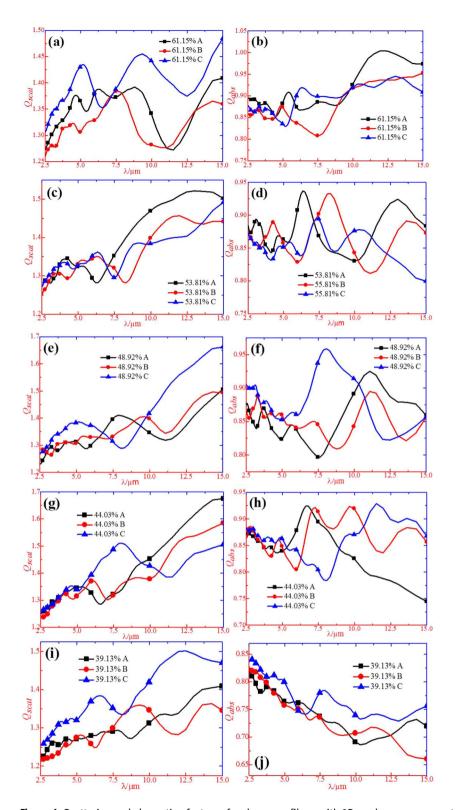


Figure 6: Scattering and absorption factors of carbon nanofibers with 2D random arrangements as a function of wavelength: (a) and (b) at a content of 61.15%, (c) and (d) at a content of 53.81%, (e) and (f) at a content of 48.92%, (g) and (h) at a content of 44.03% and (i) and (j) at a content of 39.13%.

when the quantity of carbon nanofibers with small deviation of the scattering and absorption factors of

interactions among carbon nanofibers can be enhanced radius is high. Therefore, there is a distinguished relative

Table 1: The average values of relative mean deviation of scattering factor in band of 2.5-15 µm

Content/%	61.15	53.18	48.92	44.03	39.13
Equal radius carbon nanofiber with random arrangement/%	1.26	1.20	2.48	1.94	1.73
Nonequal radius carbon nanofiber with random arrangement/%	1.89	1.31	1.96	1.57	1.46

carbon nanofibers, of which different quantities of small radius have an essential effect on their multiple scattering interactions.

Based on the aforementioned analytical results, the arrangement structure has a critical effect on the spectral radiation characteristics of carbon nanofibers. Tables 1 and 2 present the simulation results to present the average and relative mean deviations of the scattering and absorption factors with respect to various arrangement structures.

In comparison of the average values of relative mean deviations of randomly arranged equal radius and nonequal radius carbon nanofibers at the same wavelength in the entire band of 2.5-15 µm, Tables 1 and 2 present that the average value of relative mean deviation of the scattering and absorption coefficients of the random arrangement of equal radius carbon nanofibers is larger than those with nonequal radius, where the nanofiber contents are of 61.15% and 53.18%. Analytical results indicate that the random distribution has a greater effect on the radiation characteristics of carbon nanofibers than the number of particle sizes. When the nanofiber contents are 48.92%, 44.03% and 39.13%, the average values of relative mean deviations of the scattering and absorption factors of randomly arranged carbon nanofibers are smaller than that of nonequal radius. These analytical results reveal that the number of carbon nanofiber plays a more important role in determining the radiation characteristics than the random arrangement, where the nanofiber content is small. The number of carbon nanofibers with nonequal radius is higher than that with equal radius, where the nanofiber contents are same, resulting in the enhanced multiple scattering interactions among carbon nanofibers. Therefore, the relative mean deviations of the scattering and absorption factors of carbon nanofibers are then enhanced.

### 3.4 Comparison of the effect of arrangement structure on spectral radiation characteristics

Figure 7 plots the scattering and absorption curves for uniform and random arrangement of carbon nanofibers with contents of 61.15%, 53.18%, 48.92%, 44.03% and 39.13%. The values of the scattering and absorption factors in the uniform arrangement mode are larger than that of the random arrangement. With the nanofiber content of 39.13%, the average values of relative deviations of the scattering and absorption factors are 29.55% and 30.12%, respectively, over the entire band of 2.5-15 µm. With the nanofiber content of 61.15%, the average values of relative deviations of the scattering and absorption factors are 14.5% and 14.71%.

For the uniform arrangement of carbon nanofibers, the spacing between each nanofiber is uniform, resulting in the significantly enhanced scattering and absorption of carbon nanofibers in comparison with that of the random arrangement. The relative deviation of both the scattering and absorption factors of uniform/random arrangements increased. Therefore, the use of a uniform arrangement model instead of a random arrangement model will have a large deviation from the actual carbon nanofiber scattering and absorption factors.

### 3.5 Effect of 2D and 3D arrangements on spectral radiation characteristics

For the 3D random arrangement of carbon nanofiber, the XY plane with the Z coordinate of 0 is selected in the simulation. Figure 8 shows the scattering and absorption curves of the carbon nanofiber with 2D and 3D arrangements.

Table 2: The average values of relative mean deviation of absorption factor in band of 2.5-15 µm

Content/%	61.15	53.18	48.92	44.03	39.13
Equal radius carbon nanofiber with random arrangement/%	1.72	1.47	4.14	2.43	2.55
Nonequal radius carbon nanofiber with random arrangement/%	1.79	1.83	2.21	1.99	2.02

In the spectrum band of 2.5–15 µm, the average values of the relative deviations of the scattering factors are 10.10%, 26.87%, 60.47%, 15.21% and 15.21%, respectively, when the nanofiber contents are 61.15%, 53.18%, 48.92%, 44.03% and 39.13%. The average values of the relative deviations of the absorption factors are 6.69%, 10.89%, 17.42%, 18.91% and 18.91%. These analytical results reveal that the effects of 2D and 3D random arrangements on the spectral radiation characteristics have the similar trend with each other. At the wavelength of 10 µm, the scattering factor of carbon nanofiber reaches its peak value in the 3D random arrangement. At 2.5 um. the deviation of 44% is achieved for the 2D random arrangement in comparison with that for the 3D random arrangement. Furthermore, the deviation increased to 86% at 15 µm. These analytical results are originated from the cross sections of the 2D and 3D random arrangements. With an increase in the cross section of the 3D random arrangement, there is an increase in the spectral radiation

characteristics and the incensement is higher than that of the 2D random arrangement. Therefore, the simulation of the 3D random arrangement model provides a high accuracy to describe and predict the spectral radiation characteristics in comparison with the 2D random arrangement model.

As the projection area of the cylindrical carbon nanofiber in the 3D random arrangement is different from that in the 2D random arrangement along the light irradiation direction, both the multiple scattering and their interactions among carbon nanofibers are enhanced. Here, the scattering and absorption cross sections of carbon nanofibers in the 3D random arrangement are then increased to higher values than that in the 2D random arrangement. It should be noted that the calculation of scattering and absorption cross sections of carbon nanofibers in the 2D random arrangement becomes large compared to that in the 3D random arrangement.

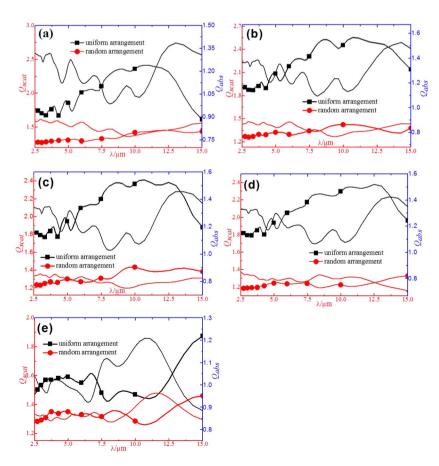


Figure 7: Scattering and absorption factor curves of carbon nanofiber in uniform and random arrangements: (a) at a nanofiber content of 39.13%, (b) at a nanofiber content of 44.03%, (c) at a nanofiber content of 48.92%, (d) at a nanofiber content of 53.18% and (e) at a nanofiber content of 61.15%.

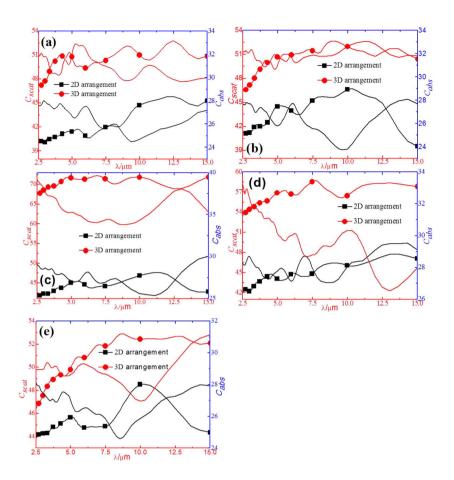


Figure 8: Scattering and absorption factors curves of carbon nanofiber in 2D and 3D arrangements: (a) at a nanofiber content of 39.13%, (b) at a nanofiber content of 44.03%, (c) at a nanofiber content of 48.92%, (d) at a nanofiber content of 53.18% and (e) at a nanofiber content of 61.15%.

### 4 Conclusion

In this study, the finite difference time-domain method is introduced to investigate the spectral radiation characteristics of carbon nanofiber in both uniform and random distributions in the spectrum band of 2.5-15 µm. The simulation results demonstrate that the spectral radiation characteristics gradually increased with an increase in the nanofiber content. The random arrangement method has a slight effect on the radiation characteristics at high nanofiber content. When the nanofiber content is reduced to the threshold value of 48.92%, the effect on radiation characteristics becomes significant. The average values and relative deviations of the scattering factor and absorption factor are 29.55% and 30.12%, respectively, using the uniform arrangement model, whereas the nanocomposite is incorporated of 39.13% nanofiber content. In comparison with the 3D random arrangement method, the analytical results of the 2D arrangement method reveal that the relative deviation of the scattering factor increased by 15.24%, while that of the absorption factor increased by 11.73%. The simulation of the 3D random arrangement model provides a high accuracy to describe and predict the spectral radiation characteristics of carbon nanofiber. This study is expected to explore the fundamental working mechanism and constitutive relationship of spectral radiation characteristics of carbon nanofiber in both uniform and random distributions.

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