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COMPUTER MODELING OF ELECTROMAGNETIC WAVE SCATTERING BY NANOCOMPOSITES CONSIDERING THE AGGREGATION EFFECT

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ABSTRACT

Background. The increase in electromagnetic pollution requires the creation of new materials that can effectively shield radiation and mitigate its negative impact. Special attention is focused on composite materials due to their ability to absorb or scatter radiation. Rayleigh theory makes it possible to predict the intensity of scattered radiation by dispersed media in the case when the particle sizes are much smaller than the wavelength. Considering the possibility of nanoparticle aggregation due to stochastic processes can increase the prediction efficiency.

Model and Implementation Tools. The proposed nanocomposite model has the shape of a cube in which spherical particles of the same radius and volume are randomly arranged. The formation of agglomerates occurred when the distance between the centers of neighboring particles did not exceed their diameter. Additionally, the interaction of particles at a small distance between them, which causes their mutual attraction, was considered. Numerical experiments were implemented in Python using NumPy libraries for vectorized computations and cKDTree for efficient spatial neighbor search.

Results and Discussion. The average values of the number of filler particles of different volumes formed as a result of random aggregation were determined in the range of filler concentrations of 0.1–7% using computational experiments. It was found that the percentage of isolated initial nanoparticles decreases with increasing filler concentration. The largest number of formations contains only two nanoparticles. It was established that the scattering of electromagnetic waves in the IR and radio frequency ranges increases due to the aggregation of nanoparticles. The size and concentration of the initial nanoparticles have different effects on the change in the scattering cross-section. The mutual attraction and coupling of closely spaced particles additionally increase the Rayleigh scattering by dispersed media.

Conclusions. An averaged distribution of the formed agglomerates in a system of spherical nanoparticles by their volume was found as a result of a series of computational experiments. Based on Rayleigh theory, it has been demonstrated that the aggregation of nanoparticles causes an increase in the scattering of electromagnetic waves by dispersed media.

Keywords: Modeling, numerical experiment, dispersed medium, nanoparticle aggregation, Rayleigh scattering.

INTRODUCTION

The widespread application of wireless communication technologies and the ubiquitous use of electronic devices are not only significantly changing our society but also causing an increase in electromagnetic pollution and potential health hazards. Besides, increasing electromagnetic interference can degrade the performance of various electronic devices. Control over growing electromagnetic interference requires the creation of new materials that can effectively shield radiation and mitigate its negative impact, while taking into account other technological demands such as high strength-to-weight ratio, flexibility, corrosion resistance, etc. [1-3]. As a result, composite radiation-absorbing materials (RAMs) have become the focus of much research due to their ability to absorb or scatter electromagnetic waves, providing a variety of functionalities [4-6]. In particular, RAMs are used to prevent electromagnetic radiation leakage in medical equipment, to develop radiation-protective clothing, to ensure the compatibility of electronic devices with respect to electromagnetic interference, to improve the performance of communication systems, and to mask objects in the microwave and infrared ranges in military applications.

Typically, composite RAMs are produced by dispersing one or more types of absorbent fillers in a polymer matrix. Fillers have dielectric and magnetic losses, the frequency dependence of which is responsible for the effectiveness of the composite in absorbing and/or scattering electromagnetic waves. An additional advantage of composite RAMs is the close relationship between their structural and functional characteristics, which allows for tuning of electromagnetic interference shielding in the required frequency range by choosing the polymer matrix and filler type. The main attention of researchers is focused on radiation-absorbing fillers such as carbon black, graphene, carbon fibers and nanotubes, as well as materials with high dielectric permittivity (oxides, titanates, etc.) and magnetic permeability (ferrites and magnetodielectrics) [7-10]. To further improve the shielding characteristics of radiation-adsorbing composites, the influence of the structure and morphology of the filler on the properties of radiation attenuation is being extensively studied [11, 12]. Electromagnetic wave scattering by such composite materials also requires additional research.

Computational methods are usually used to elucidate the mechanisms of interaction of composite materials with radiation [13-15]. Most theoretical research has focused on determining the effective properties of disordered composites from first principles, which requires significant computational resources. Mie theory and Rayleigh theory for the case where particle sizes are much smaller than the wavelength make it possible to predict the intensity of scattered radiation by dispersed media. Considering the possibility of nanoparticle aggregation due to stochastic processes can increase the forecasting effectiveness. Therefore, the purpose of the work was to find the features of electromagnetic wave scattering by disordered composites with one type of filler based on computer simulation of a system of spherical nanoparticles in a host matrix.

MODEL DESIGN

A model of a nanocomposite volume element in the shape of a cube with edge length a, in which spherical particles of the same radius R_0 and volume V_0 are randomly arranged, is proposed in the paper. The dimensions of the cube are two to three orders of magnitude larger than the dimensions of the filler nanoparticles. For clarity, the model investigated in the work corresponds to a nanocomposite film with a thickness of 5 μm and a radius of filler nanoparticles in the range of 5–100 nm, which is consistent with the case of scattering of radiation in the IR or radio frequency ranges by a thin composite coating. The model can be applied when the wavelength is at least an order of magnitude larger than the particle size. The number of nanoparticles N_0 with radius R_0 in the considered element is determined by the volume concentration of the filler C_V as

$$N_0 = \frac{C_V a^3}{V_0}. \tag{1}$$

The position of each nanoparticle in the volume element is set randomly. Their aggregation into larger agglomerates was carried out similarly to the formation of percolation clusters in the nanotube system [16]. In the case when the distance d between the centers of neighboring nanoparticles does not exceed $2R_0$, the model assumes their aggregation into a larger structure, as shown in **Fig. 1**. The nanoparticles were moved apart by a distance of double the radius for the case $d < 2R_0$ to avoid overlapping of the initial nanoparticles and a decrease in the volume of the formed agglomerate. As a result, the volume of the agglomerate formed by the aggregation of k spherical components was kV_0.

The parameter δ was additionally introduced to take into account the interatomic and/or intermolecular interaction of nanoparticles (van der Waals forces). In this case, the nanoparticles were attracted to each other under the condition $d \leq 2R_0+\delta$. The parameter δ value was in the range from 0.5 to 4 nm, which corresponds to the distances characteristic of van der Waals interactions.

A set of computational experiments was carried out for each value of concentration C_V in the 0.1–7% range and the radius R_0 of the nanoparticles in the range of 5–100 nm. As a result, the averaged distribution of the formed filler particles by their volume was found. The total number of initial nanoparticles in the volume element was in the 10^2–10^8 range and depended on their size and concentration. The effect of nanoparticle aggregation on the scattering of electromagnetic waves was investigated using the expression for Rayleigh scattering by dispersed media

$$\sigma_0 = \frac{24\pi^3 \nu V_0^2}{\lambda^4}\left(\frac{n_f^2 - n_m^2}{n_f^2 + 2n_m^2}\right)^2. \tag{2}$$

Here, σ_0 is the scattering cross-section, ν is the number of particles with the volume V_0 in a unit volume, λ is the wavelength, n_f and n_m are the refractive indices of the filler material and the host matrix, respectively. Given that the total number of initial nanoparticles in the volume element for the chosen concentration C_V and radius R_0 does not change, the change in the Rayleigh scattering cross-section due to random aggregation of nanoparticles will be determined by the expression

$$\frac{\sigma}{\sigma_0} = \frac{1}{N_0}\sum_k N_k k^2, \tag{3}$$

where N_k is the number of particles formed as a result of the aggregation of k initial nanoparticles of volume V_0.

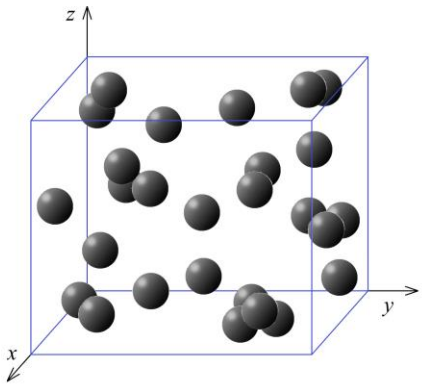


Fig. 1. Schematic representation of the composite material model taking into account nanoparticle aggregation.

IMPLEMENTATION TOOLS

The numerical experiments were implemented in Python using open-source scientific libraries such as NumPy for vectorized computations and SciPy's cKDTree for efficient spatial neighbor searches. Particle positions were generated with NumPy's random module and iteratively adjusted through custom overlap-resolution routines that operate on NumPy arrays. The cKDTree structure from SciPy was used to rapidly identify particle pairs within specified distance thresholds during each relaxation step. Cluster detection was performed through a Python implementation of the Union–Find algorithm, applied to neighbor pairs returned by cKDTree queries.

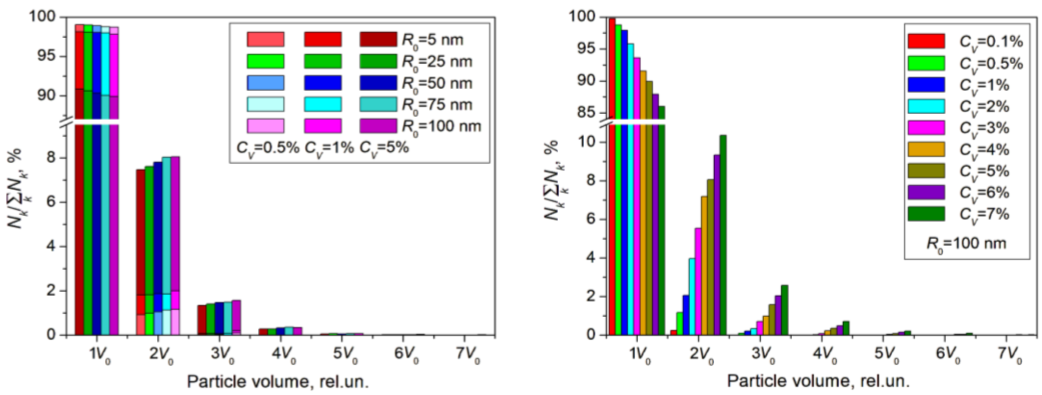
All simulations were executed over multiple concentration values and Monte-Carlo trials within a single Python workflow, producing cluster-size statistics for each scenario.

RESULTS AND DISCUSSION

The average values of the number of filler particles of different volumes formed because of random aggregation were determined through computational experiments. As can be seen in **Fig. 2**, the vast majority of the initial nanoparticles do not combine into larger aggregates and remain isolated for the investigated range of filler concentration. The fraction of isolated nanoparticles of volume V_0 is maximum (about 99.8%) for a concentration of 0.1% and decreases to 86.0% when the filler concentration increases to 7%. Conversely, the percentage of formed aggregates with a volume of $2V_0$ was increased from 0.2 to 10.3% with increasing filler concentration in the range of 0.1–7%. A similar trend was observed for particles with volumes of $3V_0$, $4V_0$, etc. Moreover, their share in the distribution decreased exponentially with increasing volume of formations. The percentage of particles with a volume exceeding $7V_0$ was less than 0.1% even for the maximum filler concentration within the study. It should be noted that the size of the initial nanoparticles had almost no effect on the distribution of the formed aggregates by their volume.

The found distribution of the number of formed filler particles by their volume made it possible to study the effect of random aggregation of the initial nanoparticles on the processes of Rayleigh scattering of electromagnetic waves by dispersed media using expression (3). **Fig. 3** shows the dependence of the ratio σ/σ_0 on the concentration C_V of the filler.

It has been established that the scattering of electromagnetic waves increases significantly due to the aggregation of nanoparticles. In particular, the ratio σ/σ_0 is exponentially increased with increasing nanoparticle concentration, which is associated with a greater number of larger formations. For a 7% concentration of nanoparticles in the host matrix, Rayleigh scattering increased by almost 1.5 times. A perceptible effect of the size of the



(a) (b)

Fig 2. Particle volume distribution for different values of the radius R_0 of the initial nanoparticles (a) and the filler concentration C_V (b).

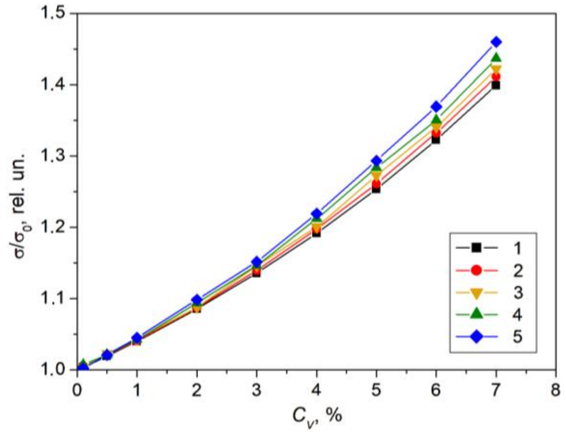


Fig 3. The dependence of the ratio σ/σ_0 on the filler concentration C_V for different values of the radius R_0 of the initial nanoparticles: 5 nm (1), 25 nm (2), 50 nm (3), 75 nm (4), and 100 nm (5).

initial nanoparticles on the aggregation-induced increase in the scattering of electromagnetic waves were observed only at a significant filler concentration. The dependencies of the ratio σ/σ_0 of the scattering cross-section on the radius R_0 of the initial nanoparticles for their various concentrations, shown in **Fig. 4**, confirm this trend. In the concentration range of 0.1–1%, no change in the value of the σ/σ_0 ratio was observed with increasing nanoparticle size, which is probably due to the small number of aggregated nanoparticles. Higher filler concentrations result in an almost linear increase in the intensity of scattered radiation with increasing R_0 compared to the case where all nanoparticles were isolated.

Consideration of the possibility of interaction of particles at a short distance between them ($2R_0 < d \leq 2R_0+\delta$), which causes their mutual attraction and the formation of larger agglomerates, is an important aspect of studying the influence of particle aggregation on the scattering of electromagnetic waves by dispersed systems. **Fig. 5** shows the dependencies of the ratio σ/σ_0 of the scattering cross-sections on the parameter δ, which determines the limiting distance of interaction between particles.

An increase in Rayleigh scattering due to the coupling of closely spaced particles was found. In particular, an increase in the limiting distance of nanoparticle interaction leads to a greater number of agglomerates and, as a consequence, an increase in the ratio σ/σ_0. In addition, the obtained dependencies are more influenced by the concentration of nanoparticles than by their radius.

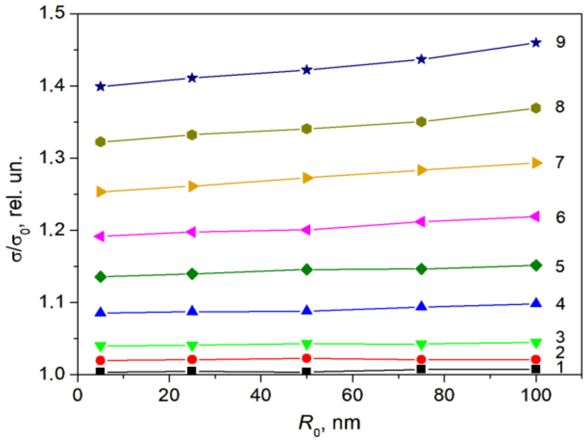


Fig. 4. Dependence of the ratio σ/σ_0 on the radius R_0 of the initial nanoparticles for different values of the filler concentration C_V: 0.1% (1), 0.5% (2), 1% (3), 2% (4), 3% (5), 4% (6), 5% (7), 6% (8), and 7% (9).

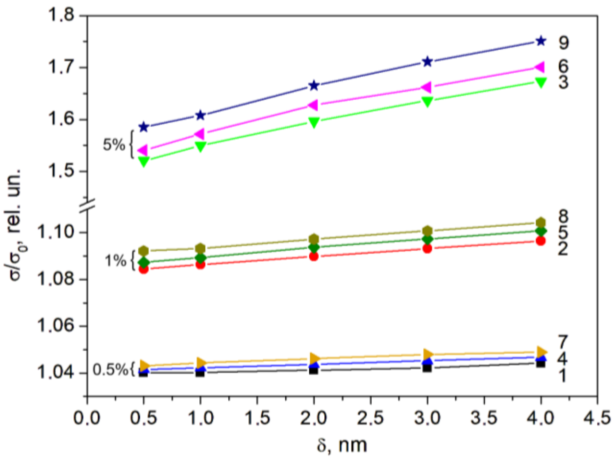


Fig 5. Dependence of the ratio σ/σ_0 on the limiting particle interaction distance *δ* for different values of the radius R_0 of the initial nanoparticles: 5 nm (1,2,3), 50 nm (4,5,6), and 100 nm (7,8,9). Curves (1,4,7), (2,5,8), and (3,6,9) related to C_V filler concentrations of 0.5, 1, and 5%, respectively.

CONCLUSION

In the work, the features of random aggregation of spherical nanoparticles in a dispersed medium were studied using computer simulation. As a result of computational experiments, an average distribution of the formed agglomerates by their volume was determined. It was established that the percentage of isolated initial nanoparticles decreases when the filler concentration increases. The formed agglomerates demonstrate the opposite trend. In addition, the share of the agglomerates in the distribution decreased according to an exponential law when their volume was increased. The radius of the initial nanoparticles has a weak effect on the distribution of the agglomerates by their volume.

Based on the numerical experiment, it was established that the scattering cross-section of electromagnetic waves in the IR and radio frequency ranges increases due to the aggregation of nanoparticles. Besides, the filler concentration has a greater effect on the aggregation-induced change in Rayleigh scattering than the radius of the initial nanoparticles. Conglutination of closely spaced particles additionally increases the radiation scattering by nanocomposites.

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COMPLIANCE WITH ETHICAL STANDARDS

The authors declare that they have no competing interests.

AUTHOR CONTRIBUTIONS

Conceptualization, [IO, YO, OA]; methodology, [IO, OS, YO]; investigation, [IO, OS, YO]; writing – original draft preparation, [IO, YO]; writing – review and editing, [IO, OA]; visualization, [YO].

All authors have read and agreed to the published version of the manuscript.

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ РОЗСІЮВАННЯ ЕЛЕКТРОМАГНІТНИХ ХВИЛЬ НАНОКОМПОЗИТАМИ З УРАХУВАННЯМ ЕФЕКТУ АГРЕГУВАННЯ

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АНОТАЦІЯ

Вступ. Збільшення електромагнітного забруднення потребує створення нових матеріалів, які можуть ефективно екранувати випромінювання та пом'якшувати його негативний вплив. Особлива увага дослідників зосереджена на композитних матеріалах, завдяки їх здатності поглинати або розсіювати електромагнітні хвилі. Теорія Релея дає змогу прогнозувати інтенсивність розсіяного дисперсними середовищами випромінювання у випадку, коли розміри частинок значно менші від довжини хвилі. Врахування можливості агрегування наночастинок внаслідок стохастичних процесів може підвищити ефективність прогнозування.

Модель і засоби реалізації. Запропонована модель нанокомпозиту має форму куба, в якому хаотично розташовані сферичні частинки однакового радіуса та об'єму. Утворення агломератів відбувалося коли відстань між центрами сусідніх частинок не перевищувала їхнього діаметра. Додатково було враховано взаємодію частинок на невеликій відстані між ними, яка зумовлює їх взаємне притягання. Числові експерименти були реалізовані на Python з використанням бібліотек NumPy для векторизованих обчислень та cKDTree для ефективного пошуку просторових сусідів.

Результати. Середні значення кількості частинок наповнювача різного об'єму, що утворилися в результаті випадкового агрегування, були визначені у діапазоні концентрацій наповнювача 0,1–7% за допомогою обчислювальних експериментів. Виявлено, що відсоток ізольованих вихідних наночастинок зменшується зі збільшенням концентрації наповнювача, а найбільша кількість утворень містить лише дві наночастинки. Встановлено, що розсіювання електромагнітних хвиль в ІЧ та радіочастотному діапазонах зростає за рахунок агрегування наночастинок. Розмір і концентрація вихідних наночастинок мають різний вплив на зміну перерізу розсіювання. Взаємне притягання і з'єднання близько розміщених частинок додатково підвищує розсіювання електромагнітних хвиль дисперсними середовищами.

Висновки. У результаті серії обчислювальних експериментів знайдено усереднений розподіл утворених агломератів у системі сферичних наночастинок за їх об'ємом. На основі теорії Релея продемонстровано, що агрегування наночастинок зумовлює збільшення розсіювання електромагнітних хвиль дисперсними середовищами.

Ключові слова: Моделювання, числовий експеримент, дисперсне середовище, агрегування наночастинок, розсіювання Релея.

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