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Mathematical Modeling of the Electrophysical Properties of a Layered Nanocomposite Based on Silicon with an Ordered Structure

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Abstract: The authors carried out modeling of the electrophysical properties of composite media. The frequency dependences of the dielectric constant on the type of inclusions in the composite are investigated. On the basis of the nanocomposite considered in the work, based on Si, B, and SiO₂, the authors model a reflecting screen, the lattice elements of which have a layered hierarchically constructed structure similar to a fractal formation. The influence of the level of fractality on the optical properties of the object was also investigated, and it was found that the proposed structure makes it possible to increase the operating frequency range of the reflecting screen and the efficiency, in comparison with reflecting screens that have a lattice of traditional structure. The results obtained can be of practical interest for broadband and nonlinear radar devices, localization devices and mobile objects, microelectronics, as well as intelligent applications in the field of information security.

Keywords: composite materials; fractional model; mathematical modeling; fractals; nonlinear dynamics; reflective screen; optical properties

1. Introduction

The increased interest of scientists, researchers, and engineers in modern composite materials is based, first of all, on a wide range of their physical and chemical properties in relation to various areas of human activity [1,2]. The prospect of using composite materials is due to many factors, the most important of which are the availability of raw materials [3] and multifunctionality [4]. Thanks to composites, the following applied problems are solved: Obtaining materials with high corrosion resistance [5], development of materials with high radioactive resistance [3], creation of new biologically compatible materials [6], synthesis of safe and environmentally friendly materials [7], microminiaturization of devices using composite media [8].

The uniqueness of composite materials lies in the fact that it is possible to design in advance the structure of the material in such a way as to give the product from it the properties necessary for solving a specific applied problem [9,10]. Material design can be one of the key factors affecting its functional properties [11]. Therefore, the determination of

the electrodynamic properties of composite media depending on the design of the material is an urgent task.

Reflective screens for passive radar reflectors and reflectors are used as elements of innovative antenna designs [12], broadband and nonlinear radar devices [13], means for localizing mobile objects [14], selective and absorbing materials [15].

There are a large number of reflective screens made, for example, in the form of a paraboloid of revolution or a solid metal plate [16]. For such reflective screens, the following disadvantages can be distinguished—they are large mass and high aerodynamic resistance. Reflective screens made in the form of a thin conductive perforated plate [17], or in the form of a system of parallel thin metal plates, the planes of which are parallel to the direction of wave propagation and perpendicular to the electric field vector [18], have a lower mass. However, the disadvantage of these screens is the leakage through them of part of the power of the electromagnetic wave. The use of a reflective screen design containing a lattice of metal conductors makes it possible to further reduce the weight. However, it was found in [19,20] that with an increase in the radiation frequency, a part of the power leaks out, which leads to a decrease in the reflection coefficient.

In this paper, we study the frequency dependences of the complex dielectric permeability of composite media consisting of a matrix with inclusions in the form of spheres and cylinders using the selection, improvement, and development of combined mathematical models of composite structures. As an example of practical application, the developed mathematical model of a reflecting screen of a fractal structure is presented. Currently, the following types of screens are known: A screen for reflector antennas, made in the form of a paraboloid of revolution made of solid metal [17], a reflecting screen made in the form of a plate of solid metal [21]. A common disadvantage of these reflective screens is their large mass since they are made of solid metal. In addition, they have great aerodynamic resistance. These flaws were not found in reflective screens made in the form of one thin conductive perforated plate [22], or in the form of a system of parallel thin metal plates, the planes of which are parallel to the direction of wave propagation and perpendicular to the vector electric field [23]. The plates of such a shield are located at a distance from each other less than half the wavelength of the operating frequency range. The disadvantage of the considered screens is that the radiation frequency increases with leakage of part of the power through it, which reduces its reflection coefficient. When it is used as a reflector of reflector antennas, the efficiency decreases, and the directional diagram of the antennas is distorted. No control reflection maxima due to changes in the thickness of the lattice elements. The proposed reflective screen contributes to an increase in the reflection coefficient in a wide frequency range, it is possible to control the maxima reflections due to changes in geometric characteristics, as well as an increasing inefficiency. The technical result is achieved by changing the design of the lattice, each lattice element is a multilayer hierarchically constructed self-similar metal-semiconductor composite and viewed as a fractal formation.

2. Materials and Methods

To simulate the electrical properties of the research object, we use the effective medium theory [24]. The essence of the effective medium model is that the system of clusters forming the composite material is considered as a kind of new medium with the same level of polarization. Thus, knowing the parameters of each of the components of the composite, their geometric shape and concentration, it is possible to determine the characteristics of the resulting composite medium as a whole. The advantage of this approach is that in order to analyze the propagation of an electromagnetic field in a composite medium, there is no need to solve Maxwell's equations at each point in space. The construction and analysis of such models are based on the solution of the electrostatics problem in a local field in a ball.

Let there be a ball with a dielectric constant ε_1 , which is surrounded by a dielectric medium with permittivity ε_2 . The local field $\bar{E}_1$ inside the ball is defined as the sum of the external field $\bar{E}_0$ and the Lorentz field $\bar{E}_d = -\left(\frac{4\pi}{3}\right)\bar{p}$, the field of the polarized sphere. The

direction of $\bar{E}_d$ depends on the ratio of ε_1 и ε_2 : $\bar{E}_1 = \bar{E}_0 + \bar{E}_d = \bar{E}_0 - \frac{4\pi}{3}\bar{p} = \frac{3\varepsilon_2}{\varepsilon_1 + 2\varepsilon_2}\bar{E}_0$, where $\bar{p} = \chi_0\bar{E}_0$ is the vector the polarization of the medium in the ball, and χ_0 is the polarizability of the sphere. Consider a medium of volume V , with a dielectric constant ε_2 , filled with spherical inclusions with a dielectric constant ε_1 . The polarization of such a substance is determined by the sum of the polarization of the spherical inclusions: $\chi = \frac{1}{V} \sum_i V_i \chi_0$, where V_i is the volume of the i -th particle, and $f_1 = \frac{1}{V} \sum_i V_i$, volumetric filling factor. The volume is characterized by the so-called effective dielectric constant ε_{eff} . Consider a composite medium consisting of a matrix and inclusions of spherical and cylindrical shapes of several types. Depending on the type, the shape of inclusions in the matrix of the composite, and the direction of the field action, within the framework of the effective medium theory, various models are given for determining the electrodynamic properties of the composite medium:

- Chaotically located spherical inclusions in the matrix [25]:

$$\varepsilon_{eff} = \varepsilon_2 \left[1 + v(\varepsilon_1 - \varepsilon_2) / \left(\varepsilon_2 + \frac{1-v}{3}(\varepsilon_1 - \varepsilon_2) \right) \right]. \quad (1)$$

- An ordered cubic system of spherical inclusions in a matrix [26]:

$$\varepsilon_{eff} = \varepsilon_2 \left[1 + 3v / \left(\frac{\varepsilon_1 + 2\varepsilon_2}{\varepsilon_1 - \varepsilon_2} - v - 1.31 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \frac{4}{3}\varepsilon_2} v^{3.33} \right) \right]. \quad (2)$$

- Chaotically located cylindrical inclusions in the matrix under the influence of the field along the axes of the cylinders [27]:

$$\varepsilon_{eff} = \varepsilon_1 \left[1 + v(\varepsilon_1 - \varepsilon_2) / \left(\varepsilon_1 + \frac{1}{2}(1-v)(\varepsilon_1 - \varepsilon_2) \right) \right]. \quad (3)$$

- Chaotically located cylindrical inclusions in the matrix under the influence of a field perpendicularly directed relative to the axes of the cylinders [28]:

$$\varepsilon_{eff} = (v - 0.5)(\varepsilon_1 - \varepsilon_2) + \sqrt{((v - 0.5)(\varepsilon_1 - \varepsilon_2))^2 + \varepsilon_1 \varepsilon_2}. \quad (4)$$

On the basis of the above models, a software package was developed [29], which makes it possible to predict the electrodynamic characteristics of the composite depending on the type of inclusions, the frequency of external influence, which is indicated in the Equations (1)–(4) by v , and the quantitative ratio of the components that make up the composite. The tabular values of the parameters for titanium dioxide and aluminum oxide were taken as the initial data. Figures 1–3 show graphs of the dependences of the complex dielectric permittivity of Si, SiO₂, and B on the frequency of the external influence in the range of 0–80 MHz.

Figures 4 and 5 show the results of computer simulation of composite media consisting of a matrix and inclusions of various types. The following quantitative ratios of the components were considered: The volume fraction of the matrix—0.9, the volume fraction of inclusions—0.1.

Figure 1. Frequency dependence of the complex dielectric constant of silicon.

Figure 2. Frequency dependence of the complex permittivity of boron.

Figure 3. Frequency dependence of the complex dielectric constant of silicon dioxide.

Figure 4. Frequency dependences of the complex permittivity for cylindrical and spherical inclusions B in a matrix Si.

Figure 5. Frequency dependences of the complex permittivity for cylindrical and spherical SiO₂ inclusions in a matrix Si.

3. Results

The work presents the developed mathematical model of the reflecting screen of fractal structure (Figure 6). The proposed structure of the screen makes it possible to increase

the reflection coefficient in a wide frequency range with the possibility of controlling the reflection maxima by changing the geometric parameters of the structural elements.

Figure 6. Reflective screen of fractal structure.

The period of the lattices, the distance between the lattices, the length and width of the lattice element are selected from the condition [30]:

$$\cos\left(\frac{2\pi d f_{\max}}{c}\right) + \frac{c}{2b f_{\max} \ln\left(\frac{b}{\sqrt{m^2 + n^2 + p^2}}\right)} \sin \frac{2\pi d f_{\max}}{c} = 1. \quad (5)$$

where b —lattice period; n, m, p —length, width and height of a lattice element, d —distance between lattice elements, $f_{\max}$ —the maximum frequency of the operating frequency range of the screen, c —speed of light in vacuum, L —reflective screen length.

Each lattice element is a multilayer hierarchically constructed composite consisting of a metal and a semiconductor, which has a self-similar structure and is considered a fractal formation (Figure 7).

Figure 7. Reflective screen lattice element.

The minimum width of an element of a layer of a composite of a fractal structure can reach a size equal to the van der Waals radius of a chemical element of which the composite is composed.

The total number of lattice elements is chosen from the condition:

$$m = \frac{W^2}{4Fd} \quad (6)$$

where W —lattice width, F —reflector's focus.

The calculation of the reflection coefficient R of the screen was carried out as follows. The values of the reflection coefficient R for a semi-infinite medium are determined from the relation given in [31]:

$$R = \frac{(N - 1)^2 + \chi^2}{(N + 1)^2 + \chi^2} \quad (7)$$

where n and χ —refractive and absorption indices of the medium, respectively.

The refractive and absorption indices included in Expression (1), as shown by the electrodynamic calculation, satisfy the following relations [30,31]:

$$\chi = \frac{c}{2\pi df} \operatorname{arcosh} \left[\cos \frac{2\pi df}{c} + \frac{c}{2bf \cdot \ln \left[\frac{b}{\sqrt{m^2 + n^2}} \right]} \sin \frac{2\pi df}{c} \right] \quad (8)$$

$$N = \frac{c}{2\pi df} \arccos \left[\cos \frac{2\pi df}{c} + \frac{c}{2bf \cdot \ln \left[\frac{b}{\sqrt{m^2 + n^2}} \right]} \sin \frac{2\pi df}{c} \right] \quad (9)$$

where f —frequency of the operating frequency range of the screen, b —lattice period, d —distance between lattice elements, n, m —length and width of a lattice element.

Figure 8 shows a graph of the dependence of the reflection index on the frequency of the wave of external electromagnetic radiation and the level of fractality of the lattice element i (1: $i = 10$, 2: $i = 6$, 3: $i = 3$), corresponding to the following parameters of the reflective screen

- 1— $b = d = 0.5$ cm; $m = n = p = 0.5$ cm;
- 2— $b = d = 0.5$ cm; $m = n = p = 0.045$ cm;
- 3— $b = d = 0.5$ cm; $m = n = p = 10^{-2}$ cm;
- $P = i\Delta$.

Figure 8. The graph of the dependence of the reflection index on the frequency of external electromagnetic radiation and the level of fractality of the lattice element.

The proposed device works as follows. Radiation falls on a reflecting screen. With the specified parameters, the reflection coefficient $R \geq 0.99999$ for $f \leq f_{\max}$.

As can be seen from Figure 8, the operating frequency range depends on the level of fractality of the lattice element of the reflecting screen. The fractal structure of the elements of the reflecting screen allows an increase in the operating frequency range by an average of 5 GHz in comparison with the known reflecting screens with a traditional grating structure. By changing the level of fractality, it becomes possible to control the maxima of the reflection coefficient.

4. Conclusions

In this work, the frequency dependences of the real and imaginary components of the effective dielectric constant of composite media consisting of a matrix and inclusions of spherical and cylindrical shapes are obtained. The dependences of the complex dielectric constant on the frequency of the external action of the electromagnetic field in the range of 1–80 MHz of the composite of the following types of inclusions

- chaotically located spherical inclusions in the matrix;
- ordered cubic system of spherical inclusions in the matrix;
- randomly located cylindrical inclusions in the matrix under the influence of the field along the axes of the cylinders;
- close-packed cylindrical inclusions in the matrix under the influence of a field perpendicularly directed relative to the axes of the cylinders;
- randomly located cylindrical inclusions in the matrix under the influence of a field perpendicular to the axes of the cylinders.

The results obtained indicate that the structural features of the composite have a significant effect on the electrodynamic properties of the object under study. As shown by the type of inclusions, electrical layers on the boundary surfaces of dispersed particles significantly affect the complex dielectric constant.

Moreover, a model of a reflecting screen of a fractal structure was proposed in the work. If the proposed reflective screen is made with the parameters described in the article, then its efficiency, in comparison with a reflective screen with a traditional grating structure, will be increased by 5.5%.

In the future, the authors plan to continue research by conducting a full-scale experiment for the described model of the screen, as well as to continue modeling the reflecting screens of the fractal structure of other modifications.

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