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MODELING OF AN ELECTROMAGNETIC RESPONSE OF SINGLE-LAYER NANOCOMPOSITE COATINGS

The spectral characteristics of the electromagnetic response of single-layer nanocomposite coatings based on metal-dielectric structures in the optical range $\lambda = 0.2 - 1.1$ μm are calculated. Effective permittivity is determined based on the approximation of the effective environment. A comparative analysis of electromagnetic response of model nanocomposite structures calculated based on experimental values of optical parameters of nanosized nickel particles and values of nickel in a macroscopic volume with experimental results was carried out. It is shown that taking into account the experimental values of the electromagnetic parameters of nanosized metal particles increases the accuracy of prediction of the electromagnetic response of nanocomposite metal-dielectric structures.

Keywords: nanocomposite coatings, electromagnetic response, metal-dielectric structures, numerical modeling.

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МОДЕЛЮВАННЯ ЕЛЕКТРОМАГНІТНОГО ВІДГУКУ ОДНОШАРОВИХ НАНОКОМПОЗИТНИХ ПОКРИТТІВ

Розраховані спектральні характеристики електромагнітного відгуку нанокомпозитних одношарових покриттів на основі металодіелектричних структур в оптичному діапазоні $\lambda = 0{,}2 - 1{,}1$ мкм. Визначена ефективна діелектрична проникність на основі наближення ефективного середовища. Проведено порівняльний аналіз електромагнітного відгуку модельних нанокомпозитних структур розрахованих на основі експериментальних значень оптичних параметрів нанорозмірних частинок нікелю та значень, які характерні нікелю в макроскопічному об'ємі з експериментальними результатами. Показано, що врахування експериментальних значень електромагнітних параметрів нанорозмірних частинок металів підвищує достовірність прогнозування електромагнітного відгуку нанокомпозитних металодіелектричних структур.

Ключові слова: нанокомпозитні покриття, електромагнітний відгук, металодіелектричні структури, чисельне моделювання.

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МОДЕЛИРОВАНИЕ ЭЛЕКТРОМАГНИТНОГО ОТЗЫВА ОДНОСЛОЙНЫХ НАНОКОМПОЗИТНЫХ ПОКРЫТИЙ

Рассчитаны спектральные характеристики электромагнитного отклика нанокомпозитных однослойных покрытий на основе металлодиэлектрических структур в оптическом диапазоне $\lambda = 0{,}2 - 1{,}1$ мкм. Определена эффективная диэлектрическая проницаемость на основе приближения эффективной среды. Проведен сравнительный анализ электромагнитного отклика модельных нанокомпозитных структур рассчитанных на основе экспериментальных значений оптических параметров наноразмерных частиц никеля и значений, характерных никелю в макроскопическом объеме с экспериментальными результатами. Показано, что учет экспериментальных значений электромагнитных параметров наноразмерных частиц металлов повышает достоверность прогнозирования электромагнитного отклика нанокомпозитных металлодиэлектрических структур.

Ключевые слова: нанокомпозитные покрытия, электромагнитный отклик, металлодиэлектрические структуры, численное моделирование.

Problem statement. Analysis of recent researches and publications

The rapid development of modern science and technology necessitates the research and development of new materials with given electromagnetic properties [1-4].

Applied application of such materials is constantly expanding, covering such areas as electronics, information technologies, optoelectronics, power engineering and others. Of particular interest is paid to the development antireflection and selective coatings for renewable energy converters, multifunctional coatings [5-9]. For example, multifunctional coatings have the functions of shielding electromagnetic radiation in the microwave range and at the same time are transparent in the visible region of the spectrum [10].

Analysis of scientific and technical literature shows that for solving such problems, mainly used multilayer interference structures [8]. In particular, multilayered interference structures consist of alternately placed thin metal layers, and dielectrics that transparent in the visible and infrared electromagnetic radiation range. However, such structures have drawbacks, namely: the complexity of manufacturing technology and precision control of multilayer structures; insufficient mechanical strength; degradation of parameters, etc. [8, 11].

A promising option for solving these problems is the use of metal-dielectric composite materials containing nanoscale metal inclusions, which are distributed in the dielectric matrix. By varying the material and microstructure of the matrix and the filler, it is possible to change the electrophysical properties of the composite [6-8]. Multifunctional coatings based on nanocomposite materials have better characteristics than traditional multilayer structures.

However, many material and methodological issues related to the design and manufacture of such systems remain unresolved. Not received sufficient coverage of the influence of the properties of nanosized inclusions and the material of the dielectric matrix on the electromagnetic response of the entire structure as a whole [12, 13].

From the point of view of the properties of nanosized metal inclusions, it is important that the reduction of their size below a certain value, the electrophysical parameters (electric polarizability α, permittivity ε, etc.) become dimensionally dependent and differ from the corresponding characteristics of the metals in the macroscopic volume [3, 14]. At the same time, the mechanisms of optical absorption in such metal-dielectric structures are insufficiently studied. In particular, the role of the dimensional dependences of the optical parameters of metal inclusions in the absorption of nanocomposite structures has not yet been clarified [9, 12]. It should be noted that the experimental data on the optical properties of nanoscale metal inclusions are extremely limited [14, 15]. Therefore, as a rule, applied and fundamental tasks for the development of nanocomposite structures and optimization of their characteristics are solved provided that the electrophysical parameters of the nanosized metal inclusions are identical to their values in macroscopic volume [3, 5, 9]. Between the calculated and experimental optical parameters of nanocomposite structures there are often significant differences [3, 15], which raises the question of the adequacy of their prediction.

These problems can be solved by modeling the electromagnetic response of nanocomposite structures using models that take into account the properties of nanosized components.

Purpose of the study

The purpose of this work is the numerical modeling of the spectral characteristics of the electromagnetic response of single-layer coatings on the basis of nanocomposite metal-dielectric structures using the proposed model that taking into account the electromagnetic parameters of its components.

Presentation of the main research material

Modeling of spectral characteristics of electromagnetic response of single-layer coatings

To modeling the electromagnetic response of single-layer nanocomposite coatings, an improved model based on the approximation of the effective environment [16] and the phenomenological theory of optical properties of thin films was used [17].

The approximation of the effective environment establishes the connection of the effective complex permittivity of the composite $\varepsilon_{eff} = \varepsilon_{eff1} - i\varepsilon_{eff2}$ with the filling factor q and the permittivity of metal inclusions $\varepsilon_m = \varepsilon_{m1} - i\varepsilon_{m2}$ that distributed in an isotropic matrix with permittivity ε_d.

Using an approximation of the effective environment for nanocomposite metal-dielectric structures involves a number of restrictions [16]:

- metal inclusions have the shape of the sphere;
- size of the metal inclusions is much smaller than the length of the electromagnetic wave λ;
- nanosized metal component is randomly distributed in the material of the dielectric matrix.

In the case of nanosized metal inclusions that distributed on a dielectric substrate, the filling factor is determined by the microstructural parameters, namely, the average diameter D_0 and the surface concentration N_s of nanosized metal inclusions. And it is defined by the expression [17]:

$$q = \pi \frac{D_0^2}{4} N_s \tag{1}$$

In the case of Bruggheman approximation, the expression of an effective complex permittivity of the composite has the form [16]:

$$\varepsilon_{eff} = \frac{\varepsilon_m \varepsilon_d + 2\varepsilon_m (q\varepsilon_m + (1-q)\varepsilon_d)}{2\varepsilon_m + q\varepsilon_d + (1-q)\varepsilon_m} \quad (2)$$

In the approximation of the effective environment, there is no connection with the response of the metal-dielectric structure to the external electromagnetic influence. Therefore, in the model that used in this paper, phenomenological theory of optical properties of thin films is applied, which connects the parameters of the structure with its response to the electromagnetic influence. This theory is applied with the following restrictions:

- normal fall of a plane electromagnetic wave to the surface of the film structure;
- surface dimensions of the film structure are much larger than the length λ;
- thickness of the film structure is less than λ;
- absorbing film with a complex index of refraction $n^* = n - ik$ that deposited on substrate that transparent in the optical range of the spectrum.

Under these restrictions, the expressions for the transmission coefficients *T*, the reflection from the side of the film *R* and the substrate *R′*, absorption *A* can be written as follows [17]:

$$T = \frac{16 n_1 n_2 (n^2 + k^2)}{\rho \tau e^{k\gamma} + æ\sigma e^{-k\gamma} + 2s\cos n\gamma + 2t\sin n\gamma}, \quad (3)$$

$$R = \frac{æ\tau e^{k\gamma} + \rho\sigma e^{-k\gamma} + 2q\cos n\gamma + 2r\sin n\gamma}{\rho\tau e^{k\gamma} + æ\sigma e^{-k\gamma} + 2s\cos n\gamma + 2t\sin n\gamma}, \quad (4)$$

$$R' = \frac{\sigma\rho e^{k\gamma} + \tau æ e^{-k\gamma} + 2q\cos n\gamma - 2r\sin n\gamma}{\rho\tau e^{k\gamma} + æ\sigma e^{-k\gamma} + 2s\cos n\gamma + 2t\sin n\gamma}, \quad (5)$$

$$A = 1 - T - R, \quad (6)$$

where

$æ = (n - n_1)^2 + k^2$; $\rho = (n + n_1)^2 + k^2$;

$s = (n^2 + k^2)(n_1^2 + n_2^2) - (n^2 + k^2) - n_1^2 n_2^2 + 4 n_1 n_2 k^2$;

$q = (n^2 + k^2)(n_1^2 + n_2^2) - (n^2 + k^2) - n_1^2 n_2^2 - 4 n_1 n_2 k^2$;

$\sigma = (n - n_2)^2 + k^2$;

$r = 2k(n_2 - n_1)(k^2 + n^2 + n_1 n_2)$;

$\tau = (n + n_2)^2 + k^2$;

$t = 2k(n_2 + n_1)(k^2 + n^2 - n_1 n_2)$;

$\gamma = \frac{4\pi d}{\lambda}$;

n – refractive index of the substrate;
k – absorption index of the substrate;
n_1 i n_2 – respectively, the refractive index of air and substrate.

In this case, the complex permittivity is related with *n* and *k* by expressions: $\varepsilon_1 = n^2 - k^2$, $\varepsilon_2 = 2nk$.

Thus, the proposed model establishes the relationship between the electromagnetic response of a nanocomposite single-layer structure with electromagnetic and microstructural parameters of its components.

The object of the modeling is a single-layer nanocomposite coating in the form of monolayer nanosized metal inclusions that deposited on a dielectric substrate. As a dielectric substrate, fused quartz, which has a window of transparency from the near ultraviolet to the near-infrared region of the spectrum, is chosen. As a metal component, nickel is selected, since it is used to solve a number of tasks.

In the case of nanocomposite coatings in the form of monolayers of nanosized metal inclusions on a dielectric substrate, the value of the permittivity of the environment ε_a, which contains metal inclusions, is determined by the expression [18]:

$$\varepsilon_a = \frac{1 - n_2^2}{2} \tag{7}$$

Examples of the results of calculations of the spectral dependences of the real and imaginary part of the effective permittivity of the model composite coating based on expressions (1) - (2) are shown in Fig. 1.

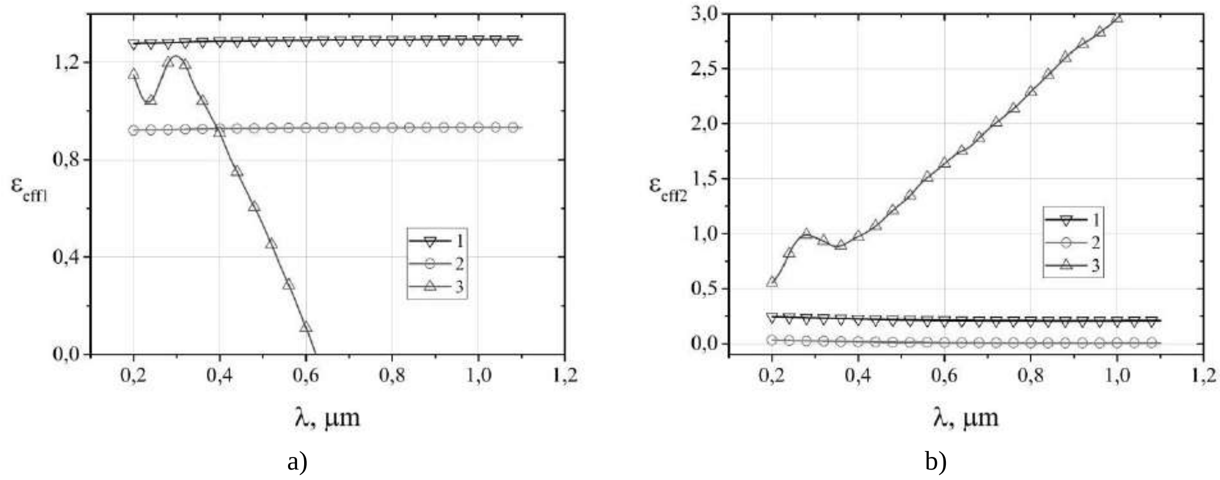

Fig. 1. Spectral dependences of the real (a) and imaginary (b) parts of the complex permittivity of the model composite coatings: 1 – $\varepsilon_a \approx 1{,}63$; 2 – $\varepsilon_a = 1$; 3 – values of ε are characteristic of Ni in macroscopic volume

Modeling was carried out under different conditions. In the first case, the value of the dielectric environment, which surrounds the nanoinclusion of nickel, was calculated by the formula (7), in the second – taken equal to one. Experimental values of electromagnetic parameters of nanosized nickel particles of D_0 = 5 nm that present in [14] were used as values of the permittivity of metal inclusions. For comparison in Fig. 1 shows the spectral dependences of the real and imaginary parts of the complex permittivity of model composite coatings that calculated from the values of optical parameters characteristic of nickel in macroscopic volume [19].

The results of numerical modeling of the spectral characteristics of response of the nanocomposite coating on the example of its absorption coefficient *A* are shown in Fig. 2.

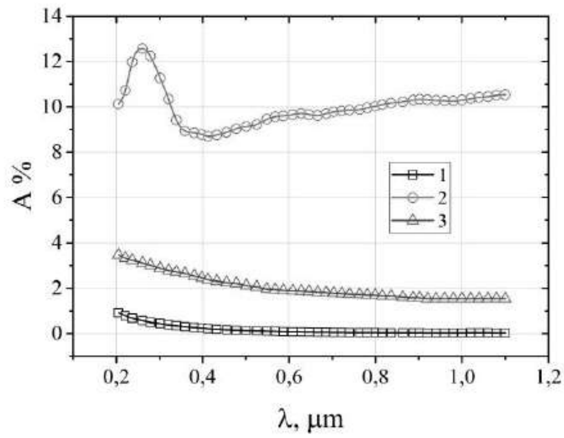

Fig. 2. Spectral Dependences of absorption coefficient: 1 – model composite coating calculated on the basis of experimental values of electromagnetic parameters of nanosized particles of Ni; 2 – model composite coating calculated on the basis of values of characteristic Ni in macroscopic volume; 3 – experimental curve for composite coatings in the form of nanosized film of Ni with a weight thickness of 0.9 nm that deposited on the dielectric substrate

It can be seen that the spectral dependence of the absorption coefficient of the model coating that calculated based on the experimental values of the electromagnetic parameters of the nanosized nickel inclusions correlates with the experimental curve. In turn, the spectral characteristic for a model nanocomposite coating that calculated on the condition that the optical parameters of the metal nanoinclusion have values are characteristic of macroscopic volumes of metal significantly differ from the experimental curve. This confirms the expediency of using experimental optical parameters of nanosized metal inclusions to predict the electromagnetic response of nanocomposite structures.

Conclusions

The model of electromagnetic response of single-layer nanocomposite coatings is presented, taking into account electromagnetic and microstructural parameters of their components. Taking into account the reliable experimental values of the parameters of the metal nanoinclusions when calculating the response of nanocomposite metal-dielectric coatings to external electromagnetic influence increases the accuracy of the obtained results. Thus, the necessity of studying the electromagnetic properties of metals in the nanosized phase is shown in order to increase the accuracy of prediction of the electromagnetic response of nanocomposite metal-dielectric coatings. Research results are of interest for the development and optimization of single-layer composite coatings and functional devices based on them with given electromagnetic characteristics.

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