Materials Physics and Mechanics 39 (2018) 87-91 Received: November 1, 2017

INTERACTION OF OPTICAL WAVES WITH A SCREENING THIN-FILM ALUMINUM COATING HAVING NICKEL NANOPARTICLES

T.M. Pechen*, A.M. Prudnik

Belarusian State University of Informatics and Radioelectronics, P. Brovka 6, 220013, Minsk, Belarus

*email: tat@bsuir.by

Abstract. Simulation of interaction of the optical waves (200...1000 nm) with nanostructure aluminum-nickel thin-film shields in the program CST Studio Suit is presented. Relationships between optical properties, substrate temperature and film composition are found.
Keywords: absorption, nanoparticle, reflection, thin film, ultraviolet region, wavelength

1. Introduction

Nanomaterials are widely used in different branches of science and technology: optics, power engineering, photo-electrochemistry, electronics, medicine and others. Thin films of nanometer sizes are used in luminescent materials, in solar batteries, in colorants with special properties, in mini sensors for adsorption of gases, in gas sensors, in explosives, etc. [1].

Thin films can be obtained by physical and chemical methods. The most popular of these are vacuum deposition, ion-beam sputtering, sol-gel method, thermal evaporation, chemical vapor deposition, spray pyrolysis of aerosols. The last noted method is one of the simple and economic. It is important that when thin films are obtained by pyrolysis, light alloying of any element in the corresponding fractions is ensured. This method is convenient to use when it is necessary to produce a homogeneous surface of thin films of highly required thickness and fully dense material [2].

The method of aerosol pyrolysis spray can be used for metal oxides, semiconductor oxides, superconducting thin films, binary and triple chalcogenides. The deposition velocity, the substrate temperature, the air pressure, the distance between the nozzles and the template are the main parameters that can be varied in this method. The ideal condition for the preparation of a film is the case when the droplets are completely removed from the solvent. In Ref. [3] the mathematical model of evaporation of micro- and nanosized drops is given, which allows to determine whether the particles will be filled or hollow.

Thin films, which represent a two-component structure of the absorber-reflector type, are at present the most common. Aluminum is a good absorber (absorption coefficient is more than 0.7, and the reflection coefficient is less than 0.3) in the ultraviolet range of wavelengths. The reflection coefficient of nickel in this range is higher [4]. Therefore, the investigation of the optical properties of the aluminum-nickel nanomaterial is a priority.

2. Interaction of electromagnetic waves with nanoparticles

Different numerical methods allow analyzing the interaction of electromagnetic waves with nanoparticles. Method classification, as a rule, is carried out depending on the way of solution. The most known methods are:

1) Finite differences in the time interval (FDTD),
2) Finite elements (FE),

http://dx.doi.org/10.18720/MPM.3912018_14

3) Final integration (FIT),

4) Moments (MoM),

5) Integral equations.

Software for solving such problems in the optical range is developed by the following companies: Rsoft FullWaVE, Optiwave OptiFDTD, EM Explorer Studio, EM Photonics FastFDTD, COMSOL Multiphysics. In Ref. [5] the analytical review of software products of the specified manufacturers is presented. From the point of view of the simplicity and convenience of modeling we chose CST Studio Suit, which is developed on the basis of the finite integration method (FIT) by Computer Simulation Technology (CST).

Consider briefly the main provisions of the program CST Studio Suit, used for modeling [6]. Numerical solution of Maxwell's equations is realized in an integral form, and not in a differential one. To determine the final area of calculations, the computational domain (interval) is divided into a set of grid cells shown in Fig. 1 The spatial discretization of Maxwell's equations is established on two orthogonal grid systems (two rightmost extreme elements). For each grid, element Maxwell's equation is formulated:

$$\int \vec{E} \cdot \overrightarrow{dS} = -\frac{\partial}{\partial t} \iint \vec{B} \cdot \overrightarrow{dA}. \tag{1}$$

For further calculations, Faraday's law is applied and equality (1) is rewritten as follows:

$$e_i + e_j - e_k - e_l = -\frac{\partial}{\partial t} b_n. \tag{2}$$

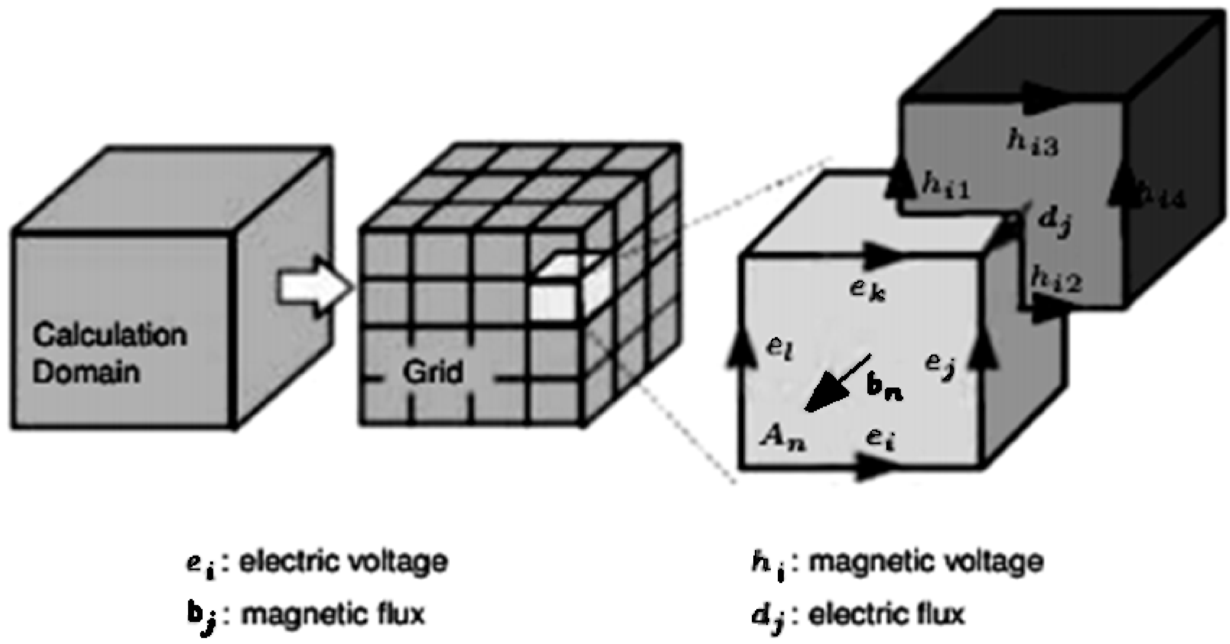


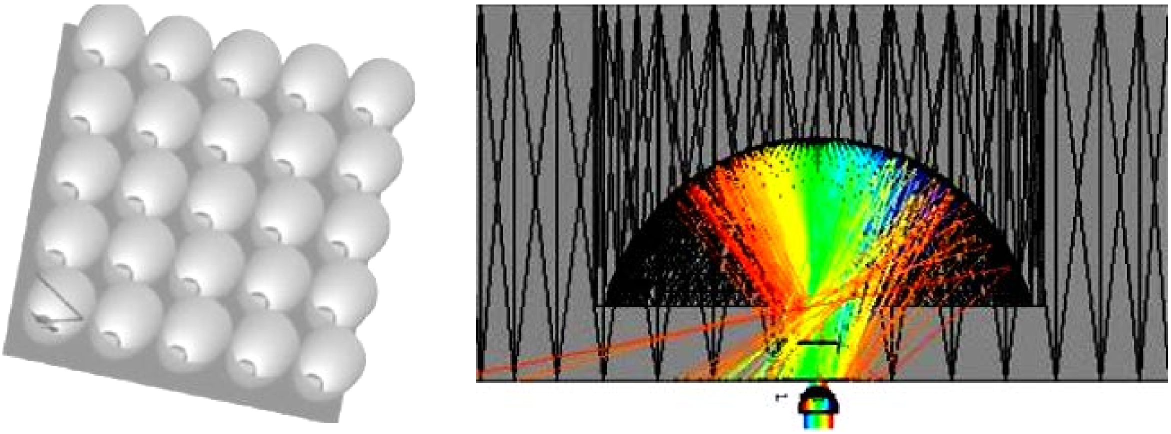
Fig. 1. Graphical interpretation of the finite iteration method (FIT)

It is important that in CST Studio Suit one can specify different properties of multilayer materials: the properties of conductors, metals with losses, dispersion materials, coatings with surface impedance and others. Fig. 2 shows:

a) Model of coating under investigation;

b) Image fragment of simulating the interaction of the EMW with the material studied.

To our mind the program CST Studio Suit is the most optimal for modeling in the optical wavelength range.



a) Appearance of coating b) Fragment of a model element studied

Fig. 2. Image of a modeled object in CST Studio Suit

3. Results and discussion

The task was to establish the relationship between the optical properties and the substrate temperature and the ratio of the film components, i.e. aluminum (Al) and nickel (Ni).

The coating optical properties are characterized by two main coefficients: absorption and thermal emissivity, which are calculated by formulas (3) and (4) respectively [7]:

$$\alpha_s = \frac{\int_{0,3}^{0,4} I_s(\lambda)\cdot[1-R(\lambda)]d\lambda}{\int_{0,3}^{0,4} I_s(\lambda)d\lambda}, \tag{3}$$

$$\varepsilon_t = \frac{\int_{250}^{1000} I_b(\lambda,\mathrm{T})\cdot[1-R(\lambda)]d\lambda}{\int_{250}^{1000} I_b(\lambda,\mathrm{T})d\lambda}, \tag{4}$$

where $I_s(\lambda)$ is the radiation intensity of the spectral range of the sun regulated by [8], $R(\lambda)$ is the material reflection coefficient measured at a specific wavelength λ, $I_b(\lambda,\mathrm{T})$ is the radiation intensity of an absolutely black body; T is a temperature.

The optical properties of the coatings under investigation depend on the temperature so it was decided at first to study a coating of nickel (60%) and aluminum (40%) at different temperatures (300 ... 550°C). The absorption coefficient values are given in Table 1. As can be seen the absorption coefficient has the maximum at temperature T = 400°C, and the minimum at T = 500°C. Afterwards the reflection coefficient was investigated at various temperatures from ultraviolet wavelengths to near infrared ones (200 ... 1000 nm). Figure 3 shows the results obtained. As can be seen the reflection coefficient for the UV region does not exceed 25%, and it is less than 5% at 400°C. Therefore there is the possibility of using this coating at the indicated temperature. In the visible and near-IR regions, the reflection coefficient varies little (almost constant): its value is 40% and 10%.

Then the absorption coefficient of this coating (60%Ni-40%Al) was investigated at various temperatures from ultraviolet to near infrared (200 ... 1000 nm). In Fig. 4 the results obtained are shown. At the last stage of investigation we have tried to establish the regularities in the influence of different contents of nickel and aluminum samples on coating optical properties. Using (3) and (4), the absorption coefficients (α_s) and thermal emissivity (ε_t) were calculated, the results are given in Table 2. As can be seen, the screen of

60% nickel and 40% aluminum is characterized by the lowest thermal emissivity, however increasing the nickel content in the coating leads to a significant growth of this characteristic.The results obtained at this stage showed that this nickel content is optimal for low reflection coefficient in the ultraviolet region.

Table 1. Coating absorption coefficients (60Ni-40 Al)

No	Temperature, °C	Absorption coefficient
1	300	0.86
2	350	0.77
3	400	0.87
4	450	0.79
5	500	0.69
6	550	0.72

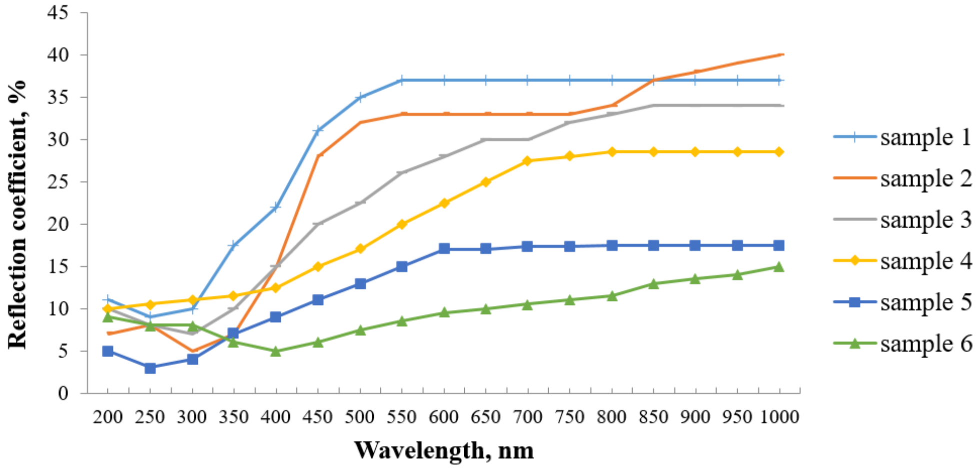


Fig. 3. Dependence of the reflection coefficient of a coating (60%Ni-40%Al) on a wavelength in the optical wavelength range at different temperatures: 1) 500, 2) 550, 3) 350, 4) 450, 5) 300, 6) 400°C

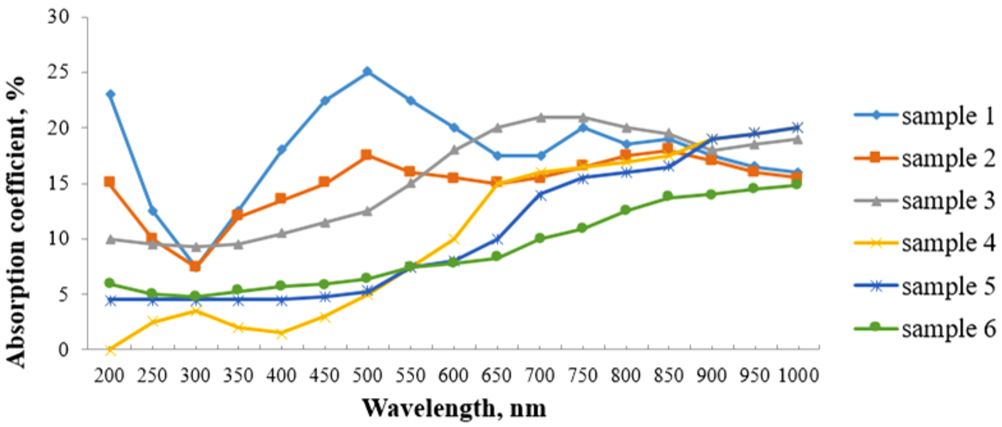


Fig. 4. Dependence of the absorption coefficient of a coating (60%Ni40%Al) on a wavelength in the optical wavelength range at different temperatures:
1) 500, 2) 550, 3) 350, 4) 450, 5) 300, 6) 400°C

Table 2. Characteristics of nickel-aluminum coatings

No	Ratio nickel / aluminum	Absorption coefficient	Thermal emissivity
1	10/90	0.81	0.29
2	20/80	0.83	0.19
3	40/60	0.80	0.35
4	60/40	0.89	0.08
5	80/20	0.85	0.40
6	90/10	0.84	0.38

The most uniform dependence of the reflection coefficient in the entire wavelength range is inherent to sample 6 (90%Ni–10%Al). The worst result is obtained for sample 1 (10%Ni−90%Al). In the ultraviolet region at the wavelength equal to 300 nm, the coefficient value is minimum (7%, and at the length of 490 nm has the maximum (25%).

4. Conclusions

We have used the program CST Studio Suit for studying the interaction of electromagnetic waves with a screening thin-film aluminum coating having nickel nanoparticles. It was found:

- Optimal content of nickel nanoparticles in the coating is 60%;
- Nonlinear character of the dependence of the reflection coefficient on a wavelength in the optical range at different temperatures;
- Thermal emissivity coefficient of the coating directly characterizes the screen reflectivity in the infrared wavelength range.

The aluminum thin-film coatings with the addition of nickel nanoparticles have a low reflection coefficient (less than 7%) in the ultraviolet region in the case of the dominant (more than 50%) component in the screen-nickel content.

References

[1] O. Kikuo, Method of preparing zinc oxide nanorods on a substrate by chemical spray pyrolysis // *Chemical Engineering Sciences* **58** (2003) 537.

[2] M. Eslamian, Modelling of nanoparticle formationduring spray pyrolysis // *Nanotechnology* **17** (2006) 1674.

[3] A.E. Nikolaenko, Carbon nanotubes in a photonic metamaterial // *Physical Review Letters* **104(15)** (2010) 153902.

[4] CST STUDIO SUITE 2012 – https://www.cst.com/Applications/Article/CST-STUDIO-SUITE-2012-System-Assembly-And-Modeling

[5] A.B. Khatibani , S.M. Rozati, Synthesis and characterization of amorphous aluminum oxide thin films prepared by spray pyrolysis effects of substrate temperature // *Journal Materials Science in Semiconductor Processing* **18** (2014) 80.

[6] Z. Li, J. Zhao, L. Ren, Quantifying regeneration in dye-sensitized solar cells // *Solar Energy Materials and Solar Cells* **105** (2012) 90.

[7] P.A. Vityaz, V.S. Urbanovich, Investigation of processes of formation of nanostructured superhard materials in conditions of high pressures on the base of refractory nitrides synthesized by SHS-method in the Ti-Al-Si-C-N-B system, In: *Materials IV International STC "NANO-2014". Minsk, October 7–10* (2014), p.10.

[8] The standard ISO 9845-1 (1992). *Solar energy – Reference solar spectral irradiance at the ground at different receiving conditions.*