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FINDING EFFECTIVE THERMAL CHARACTERISTICS OF COMPOSITE MATERIALS BASED ON THE ANALYSIS OF THERMAL CONDUCTIVITIES

This paper presents a method and algorithm for finding effective thermal characteristics of composite materials, with complex internal structure by the method of thermal-electrical analogies based on the discrete model that built for the task of analysis of the temperature field by finite element method.

Key words: composite material, thermal conductivity, thermal-electrical analogies, thermal analysis, discrete model.

Подано метод і алгоритм знаходження ефективних теплових характеристик композитних матеріалів зі складною внутрішньою структурою за допомогою методу теплоелектричних аналогій на основі дискретної моделі, побудованої для задач аналізу температурних полів методом скінченних елементів.

Ключові слова: композитний матеріал, теплопровідність, теплоелектричні аналогії, термічний аналіз, дискретна модель.

Introduction

Creating artificial materials with desired physical properties is one of the important aspects of modern production. Lack of information about the physical properties of materials and components not allows to do further scientific research or engineering calculations [1].

Creating a method which allows to calculate the properties of existing materials, and such that only have been created is an actual task, especially if we take into account the large number of substances that have not been investigated. Research of the mechanism of heat transfer should moves the front of works of creating materials with predetermined properties from the field of laboratory experiment in to the field of physical and mathematical research.

The results of investigation of effective thermal properties of composite materials can be used in the design of thermal modes of electronic equipment, which allows using computer-aided design to create effective and reliable devices [2].

Finding effective thermal characteristics are time-consuming task, which can be solved like the inverse problem of heat conduction [3], [4]. In certain cases it is possible to define empirical and semi-empirical formulas [5], and for the simple structure of materials – have resorted to the analysis of heat in their simplified quasihomogeneous models [1]. Difficulties arise when trying to find effective thermophysical properties of materials of complex structure, including composite materials, due to the significant influence of heterogeneity of the environment on the processes of heat conduction. To solve such problems conveniently use the analogy between the processes of heat conduction and electric conduction.

Properties of composite materials

Composites or composite material (CM) – a material consisting of two or more components (individual fibers or other reinforcing components and matrix that binds them), and have specific properties that differ from the total properties of its components [6].

Interest in CM is conditioned, primarily, by the need to create materials with improved operational characteristics. Therefore, the development and research of composites consists on the one hand, in improving of the structural, physical, chemical and mechanical properties of materials in accordance with the scope of their using, the other – in increasing the technological, economic and environmental performance.

Composites on functional grounds can be divided into structural materials, i.e. materials with improved set of physical and mechanical properties, and materials with special properties: the predetermined level of conductivity, optical properties and electrical properties. The latter include electrical conductivity, dielectric constant, magnetic properties [5].

CM can be characterized by topology of their reinforcing components. Topology reflects shape of the particles of dispersed phase, their size, and distribution of dispersed phase by the volume of the dispersion medium. It also includes the size of the inclusions, the distance between them, the coordinates of the centers of inclusions, the angle of orientation in space not isodimentional inclusions (i.e. inclusions with much larger size in one or two directions, such as fibers or plates). Topology of composites is the starting point of their analysis, so CM based on continuous fibers or fabrics that are oriented in the same direction, easily can be analyzed, which is not true for composites with different topology.

Effective thermal characteristics of CM

The effective thermal characteristic of the composite material is its effective thermal conductivity λ_{eff}. This ratio reflects the ability of a material to conduct heat. Experimentally it can be defined as:

$$l_{eff} = \frac{d_m}{R_T} \left[\frac{\mathrm{W}}{\mathrm{m} \cdot {}^\circ\mathrm{K}} \right] \tag{1}$$

$$R_T = \frac{\Delta T}{q} \left[\frac{\mathrm{m}^2 {}^\circ\mathrm{K}}{\mathrm{W}} \right] \tag{2}$$

where d_m – material thickness, R_T – Thermal resistance (of part of the body), ΔT – constant temperature difference between the sides of the body [7].

For the theoretical calculation of thermal conductivity of most composite materials with different structures was defined series empirical and semi-empirical formulas [5], calculations using these formulas usually contain significant errors because it takes a large number of simplifications.

Another approach to the synthesis of effective thermal characteristics of CM is to use the results of the analysis of heat transfer in the material [1], [8], i.e. the solution of the inverse heat conduction problem [3], [4].

Analysis of heat conduction problem

Any physical phenomenon, including thermal process occurs in space-time. Therefore, analytical (mathematical) research of thermal conductivity is equivalent to research of changing spatial-temporal characteristic – temperature, which is typical for this phenomenon, that is, for finding dependence [9]:

$$T = f(x, y, z, t) \tag{3}$$

where x, y, z – is the spatial coordinate in the Cartesian system, and t – is the time.

The set of instantaneous values of temperature at all points of the explored space is called the temperature field, temperature field is a scalar quantity. There are stationary when they remain constant over time, and non-stationary when they change with time, temperature fields. According to this distinguish stationary and non-stationary heat conduction problems.

Stationary problem of heat conduction (Fourier's law), in the case of the absence of internal heat sources can be written as boundary value problem [9]:

$$q = -l \nabla T, \quad l_x \frac{\partial^2 T}{\partial x^2} + l_y \frac{\partial^2 T}{\partial y^2} + l_z \frac{\partial^2 T}{\partial z^2} = 0 \tag{4}$$

where q – heat flux density (the amount of energy that flows through a unit area per unit time), l – thermal conductivity of the medium, ∇T – gradient of temperature field. Apparently, the problem of heat conduction is described by the differential equation with partial derivatives.

Except the equation for the correctness of problem conductivity it should to determine the boundary conditions. There are three main types of boundary conditions:

Boundary conditions of the first kind or Dirichlet boundary conditions, in general have the form:

$$T_A(t) = f(t) \quad (5)$$

where $T_A(t)$ – is the surface temperature of the body.

Boundary conditions of the second kind or Neumann boundary conditions, in general have the form:

$$q_A(t) = f(t) \quad (6)$$

where $q_A(t)$ – is the density of heat flux on the body surface.

Boundary conditions of the third kind, or Robin boundary conditions, in general have the form:

$$q_A(t) = a(T_A - T_\infty) \quad (7)$$

where $q_A(t)$ – is the density of heat flux on the surface of the body, a – is the heat transfer coefficient [W/m^{2o}K], T_∞ – is the ambient temperature, the boundary condition sets the convection on the boundary of the body.

Thermal-electrical analogies

Experimental methods of researching the processes of heat conduction include method of analogies. In the method of analogies research of thermal phenomenons is replaced by researching similar phenomenons, as there is often easier to make experimental research than the direct research of thermal processes. Similarity of analogous phenomenons is based on the same character of all occurring processes. Mathematically, analogous phenomenons are described by formally identical differential equations and conditions of uniqueness. However, the physical meaning and dimension of the input values in them are different.

Electrical analogy based on the formal similarity of differential equations of heat conduction with one hand and equations of electrical conduction with the other hand [8], [9].

In the field of electrostatics is known that under Ohm's law, the current density associated with the electric field, which in turn is related to the potential:

$$J = \frac{I}{A} = -s\nabla V, \quad s_x \frac{\partial^2 V}{\partial x^2} + s_y \frac{\partial^2 V}{\partial y^2} + s_z \frac{\partial^2 V}{\partial z^2} = 0 \quad (8)$$

where I – is the amperage, A – the surface area that is perpendicular to the flow of electrical current, s – a conductivity coefficient, ∇V – is gradient of formed electric field [10]. Obviously, equation (4) and (8) are similar.

Through this approach, the problem of heat conduction can be solved on the basis of analysis of the thermal circle that constructed using analogies relevant thermal and electrical elements [8], [11].

Discrete model of thermal conductivity of composite materials

For the solution of the problem of heat conduction we propose to use the discrete model of composite materials, which is built by using adaptive irregular grids [11].

The chosen discrete model is based on a representation of CM by mesh of simplex finite elements. Creation of scheme of substitution mesh to heat circuit is based on electrical analogies (4), (8).

For analysis of thermal circle is used nodal analysis – the method of calculation of electric circuits by writing a system of linear algebraic equations in which unknowns are the potentials at the nodes of the circle. As a result of applying the method is defining potentials at all nodes of the circle and, if necessary, the current in all contours [12].

In applying the nodal analysis, thermal circle is represented by a system of linear algebraic equations:

$$[K]\{U\} = \{F\} \quad (9)$$

where $[K]$ – is the influence coefficients of each node, $\{F\}$ – are coefficients of loads caused by the presence of current sources or voltage (presence of boundary conditions of heat conduction problem).

The solution of the equation system displays the temperature at the nodes of finite elements. These values we use to find the effective thermal characteristics of CM. Selected discrete model allows to calculate the heat conduction problem of composite materials with complex topology, including the heterogeneity of environment. The model has first order accuracy.

Synthesis of effective thermal characteristics of composite materials

For systems with a regular structure λ_{eff} is determined by analyzing heat transfer in the so-called elementary cell. For getting simple approximate dependencies of λ_{eff} spend discretization of modeling object to cells by isothermal and adiabatic surfaces, resulting object is represented as a set of plots with parallel and series connection of thermal resistances [1], [8]. This approach is actual if you can predict the temperature field, such when topology CM is simple, layered with homogeneous layers.

Based on thermal-electrical analogies (4), (8), derive the dependence λ_{eff} for homogeneous layers of CM in the form of a parallelepiped [8]. At *Fig.1.a* shown model of homogeneous layer of CM, where surfaces l_1 and l_2 are isothermal with temperatures t_1 and t_2, ends of layer are adiabatic. Internal heat sources are not available, the thermal conductivity of the material is l. Need to find the value of stationary heat flow that passes through this layer.

According to (2) $\Delta T = qR_T$. According to the Fourier equation (4), the temperature difference can be written as:

$$\Delta T = \int_{l_1}^{l_2} \frac{q(l)}{A\,l} dl \tag{10}$$

Here can be found the absolute value of thermal resistance:

$$R_T = \frac{1}{q_1} \int_{l_1}^{l_2} \frac{q(l)}{A(l)\, l\,(l)} dl \tag{11}$$

where $A(l)$ – analytical representation of area of isothermal surface at distance l from the origin, $q(l)$ – heat flow through isothermal surface with an area $A(l)$, q_1 – heat flow through isothermal surface with an area $A(l_1)$.

If the path of heat flow no sources or sinks of energy, both in body and on its surface, the flow q does not change its value, i.e. $q = q_1$. Provided that $l = const$ the expression (11) can be written as:

$$R_T = \frac{1}{l} \int_{l_1}^{l_2} \frac{dl}{A(l)} \tag{12}$$

Element of the length dl of the path of heat flux for surfaces of parallelepiped (*Fig.1.a*) equal $dl = dx$, and analytical expression of the isothermal surface $A_\Pi = L_1 L_2$, where L_1 and L_2 are the length and width of the surface. Then the absolute value of thermal resistance in a particular case is expressed as:

$$R_T = \frac{1}{l} \int_{l_1}^{l_2} \frac{dx}{L_1 L_2} = \frac{l_2 - l_1}{l L_1 L} = \frac{d}{l A_\Pi} \tag{13}$$

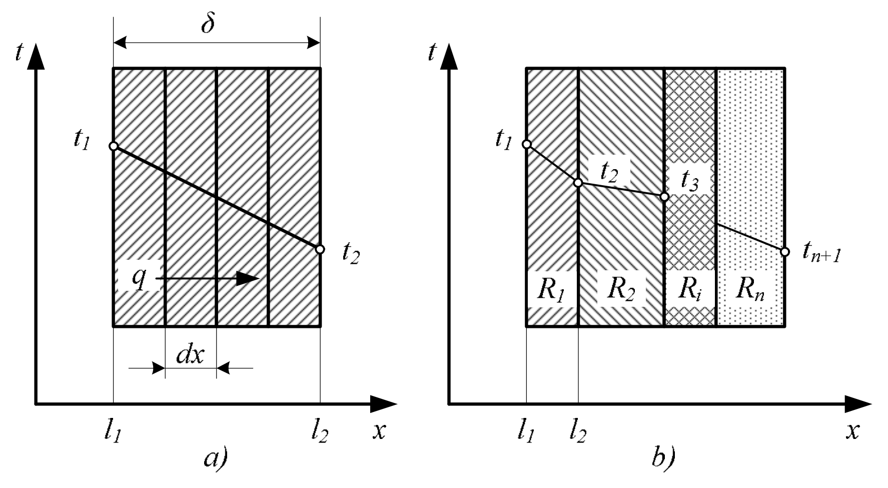

Fig. 1. Model of composite material: a – homogeneous layer; b – multilayered CM

Consider now consistently assembled CM, that consisting of n heterogeneous oriented perpendicular to the heat flow layers with thickness and thermal conductivity d_i and l_i. Temperatures of surface layers are t_i and t_{i+1} (***Fig.1.b***).

Each layer of CM can be attributed by absolute thermal resistance R_{Ti}. All absolute thermal resistances are connected in series (***Fig.1.b***), so the total absolute thermal resistance of CM will be:

$$R_T = \sum_{i=1}^{n} R_{Ti} = \sum_{i=1}^{n} \frac{d_i}{l_i A_i} = \frac{1}{A} \sum_{i=1}^{n} \frac{d_i}{l_i} \left[\frac{°\mathrm{K}}{\mathrm{W}} \right] \tag{14}$$

Let us find the expression of absolute thermal resistance for multilayered CM, with heterogeneous layers that lie parallel to the flow of heat. We must accept the assumption that heterogeneous layers are separated from each other by infinitely thin, not heat conductive (adiabatic) layer [8]. In this case the temperature field of each of the layers becomes uniform, and for each of the layers according to (10) we can determine the absolute value of thermal resistance R_{Ti}. Because the layers are parallel to the heat flux, the absolute values of the total thermal resistance of the CM is defined as:

$$\frac{1}{R_T} = \sum_{i=1}^{n} \frac{1}{R_{Ti}} = \sum_{i=1}^{n} \frac{l_i A_i}{d_i};\ R_T = d \Big/ \sum_{i=1}^{n} l_i A_i \left[\frac{°\mathrm{K}}{\mathrm{W}} \right] \tag{15}$$

Value of λ_{eff} is defined as (1), i.e. it is equal to the ratio of thickness of the CM to its thermal resistance.

Accepted assumption about the presence of adiabatic layers can significantly simplify the calculation, although in this case the question arises about the adequacy of the model, because in the case of use multilayered CM with large difference in coefficient of thermal conductivity of layers, results will be heavily distorted and do not reflect the actual physical process.

Problems of this kind are present in the calculation λ_{eff} for CM with reinforcing components like a heterogeneous inclusions or fibers. So the real heat flow replaced by a simplified by model of parallel flow lines, between which located adiabatic layers [1]. Given that the number of inclusions in the model can be very large, in case of calculation of λ_{eff} similar simplification accumulate large error.

For the synthesis of effective thermophysical properties of complex composite structures we propose to use the results of modeling of the problem of thermal conductivity (3) [13]. Discrete model (9) is based on adequate partitioning of composite by simplex finite elements, which reflect the thermal circle. According to [7], after analyzing heat conduction problem, with Dirichlet boundary conditions (5), i.e., at constant temperature on one surface of KM, and Neumann boundary conditions (6), i.e. at a constant heat flow on the opposite surface, becomes known the values of temperature at the nodes of discrete elements, and hence, becomes known surface temperature of CM.

For the synthesis the value of λ_{eff} according to (1) need to find the constant temperature difference between the surfaces of CM ΔT. As a result of simulation, the temperature on the surface may not be non-uniform, especially in cases of modeling multilayered CM with very different thermal conductivity coefficients of layers. Therefore, to find ΔT should use the model of parallel connection of resistances (15): heterogeneous surface temperature, formed at a given heat flow, describes a set of nodes of finite elements, on the opposite surface of the CM temperature is known and uniform, then each surface element reflects the absolute thermal resistance R_{Ti}, whose value is expressed as:

$$R_{Ti} = \frac{1}{n \cdot A \cdot q} \sum_{i=1}^{n} \left(T(N_i) - T_0 \right) \left[\frac{°\mathrm{K}}{\mathrm{W}} \right] \tag{16}$$

where n – number of nodes of surface element; A – surface area of the element; q – known heat flux, $T(N_i)$ – the temperature at the node of element on the surface of CM; T_0 – known temperature on the opposite surface of the CM.

According to (13) and (15):

$$\frac{1}{R_T}=\sum_{j=1}^{m}\frac{1}{R_{Tj}}=\frac{1}{L_1L_2}\sum_{j=1}^{m}\frac{1}{\frac{1}{n_j\cdot A_j\cdot q}\sum_{i=1}^{n_j}\left(T(N_i)-T_0\right)}=\frac{q}{L_1L_2}\cdot\sum_{j=1}^{m}\frac{n_j\cdot A_j}{\sum_{i=1}^{n_j}\left(T(N_i)-T_0\right)} \qquad (17)$$

where L_1 and L_2 – are length and width of surface of CM.

The temperature difference between the surfaces of the CM is expressed as:

$$\Delta T=\left(\frac{1}{L_1L_2}\sum_{j=1}^{m}\frac{n_j\cdot A_j}{\sum_{i=1}^{n_j}\left(T(N_i)-T_0\right)}\right)^{-1} \qquad (18)$$

Then, based on (1) λ_{eff} of CM defined as:

$$l_{eff}=\frac{d}{R_T}=\frac{d}{\Delta T/q}=\frac{d\cdot q}{\Delta T}=\frac{d\cdot q}{L_1L_2}\cdot\sum_{j=1}^{m}\frac{n_j\cdot A_j}{\sum_{i=1}^{n_j}\left(T(N_i)-T_0\right)}\left[\frac{\mathrm{W}}{\mathrm{m}\cdot{}^{\circ}\mathrm{K}}\right] \qquad (19)$$

Based on the results of solution heat conduction problem by discrete model (9), using (19), can be synthesized values of effective thermal characteristics of CM, General algorithm for synthesis of effective thermophysical properties of composite materials are shown in *Fig.2*.

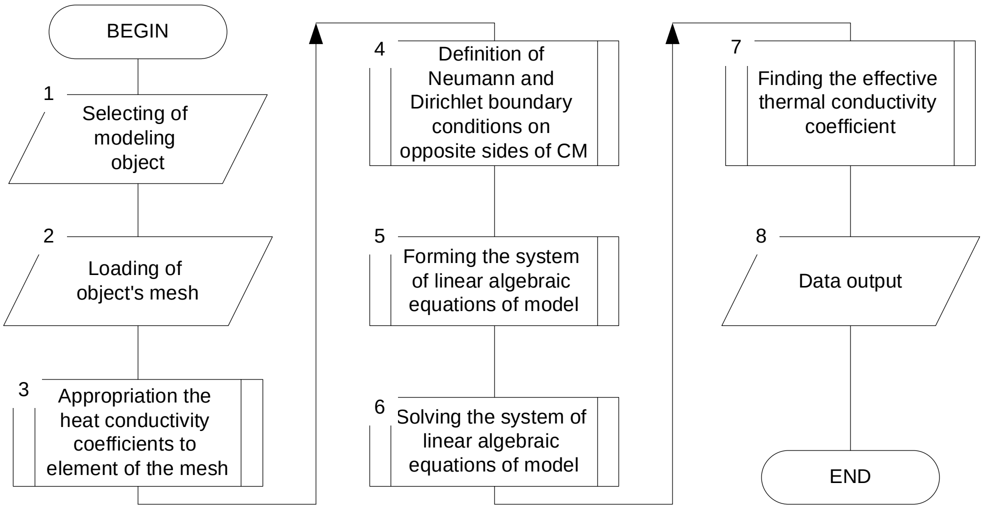

Fig.2. Algorithm for finding the effective thermophysical characteristics of CM

Example of finding the effective thermal conductivity coefficient

For example, we used the model of CM with size $2.5\cdot10^{-3}$ m (*Fig.3*), matrix of composite with coefficient of thermal conductivity 237 W/m°K (aluminum), filled with reinforcing components of spherical inclusions with radius $2.5\cdot10^{-4}$ m +/– 10^{-4} m, with a coefficient of thermal conductivity 1500 W/m°K (diamond). Transition layer between the matrix and filler has width 20 % of the radius of the inclusions, the concentration of not heat conducting material (air) in the transition layer is 10 %.

On one side of the composite defined Neumann boundary conditions – heat flux 100000 W/m$^{2\circ}$K, on opposite side defined Dirichlet boundary conditions – constant temperature 20°K.

Composite was discrete by irregular adaptive tetrahedral simplex elements mesh, the minimum angle for elements larger than $2\cdot10^{-4}$ m is 20°, number of mesh nodes is 14707, number of mesh elements is 80219. Mesh generation time on an ordinary configured computer is 122 seconds. The total computation time for ordinary configured computer is 496 seconds.

As a result of simulation was formed temperature field with maximum temperature difference 0.9076°K, and middle surface temperature difference 0.8736°K. Synthesized value of the effective thermal conductivity of composite material under given conditions is 286,163 W/m°K.

To confirm the results we conducted simulations of heat distribution in a homogeneous body with synthesized thermal conductivity, the same size and the same boundary conditions. Body discrete by tetrahedral simplex elements mesh, number of mesh nodes is 64, the number of mesh elements is 135. Mesh generation time on ordinary configured computer is less than a second. The total computation time for ordinary configured computer is $5 \cdot 10^{-3}$ seconds. As a result of simulation was formed temperature field with temperature difference 0.8736°K.

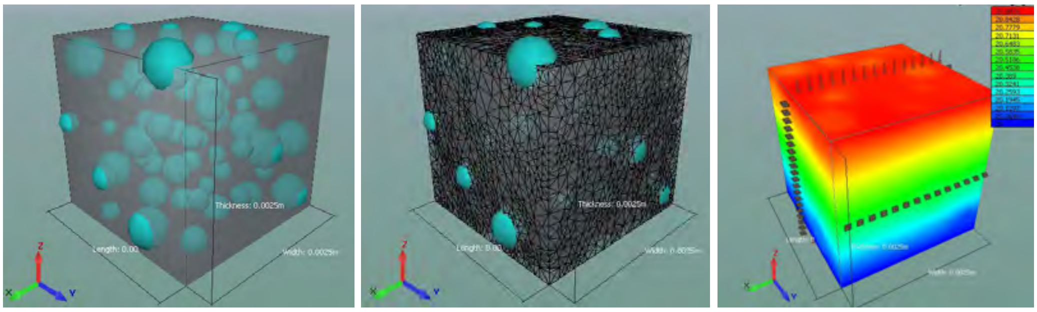

Fig.3. Example of calculating the effective thermal conductivity for composite with spherical inclusions

Conclusions

Through the analysis of heat conduction problem by using a discrete model of composite materials with using the method of thermal-electrical analogies, was developed the method and algorithm for finding effective thermophysical properties of these materials, which solves the inverse problem of heat conduction and allows conducting the calculations even for bodies with complex internal structure, avoiding real experiments.

1. Дульнев Г.Н., Заричняк Ю.П. Теплопроводность смесей и композиционных материалов: справочная книга. – Л.: Энергия, 1976. 2. Дульнев Г.Н., Парфенов В.Г., Сигалов А.В. Методы расчета теплового режима приборов. – М.: Радио и связь, 1990. 3. Алифанов О.М. Обратные задачи теплообмена. – М.: Машиностроение, 1988. 4. Lobur M., Farmaga I., Marikutsa U., Matviykiv O., Ciupinski L., Analysis and Problem Statement of the Optimal Thermal Design of Technical Objects // Proc. of the International Conference Microtechnology and Thermal, Lodz, Poland, 2011. 5. Шевченко В.Г. Основы физики полимерных композиционных материалов. – М., 2010. 6. Lubin G. Handbook of Composites // пер. с англ. А.Б. Геллера, М.М. Гельмонта. – М.: Машинострoэние, 1988. 7. ДСТУ Б В.2.7-105-2000 (ГОСТ 7076-99) Матеріали і вироби будівельні. Метод визначення теплопровідності і термічного опору при стаціонарному тепловому режимі. – К.: Видання офіційне, 2001. 8. Дульнев Г.Н. Тепло- и массообмен в радиоэлектронной аппаратуре. – М.: Высшая школа, 1984. 9. Лыков А.В. Теория теплопроводности. – М.: Высшая школа, 1967. 10. Lienhard J.H. IV, Lienhard J.H. V, A Heat transfer textbook – 3rd ed. // Cambridge, Massachusetts, 2001. 11. Farmaga I., Lobur M., Shmigelskyi P., Javorskyi N., Śpiewak P. Regular and Adaptive Meshing Algorithms for Modeling of Spherical Inclusions by Finite Element Method. // Proc. of the XI-th Intern. Conf. Modern Problems of Radio Engineering, Telecommunications and Computer Science (TCSET'2012). – February 21–24, 2012, Lviv–Slavske, Ukraine. – P. 505–507. 12. Нейман Л.Р., Демирчан К.С., Теоретические основы электротехники: Учебник для вузов. В 2-х т. – Том 1. – 3-е изд., перераб. и доп. – Л.: Энергоиздат. Ленингр. отд-ние, 1981. 13. Лобур М., Моделювання процесів теплообміну в нанокомпозитах / М. Лобур, І. Фармага, П. Шмігельський // Вісн. Нац. ун-ту "Львівська політехніка" "Комп'ютерні системи проектування. Теорія і практика". – Львів: Видавництво Львівської політехніки, 2011. – № 711. – С. 101–104.