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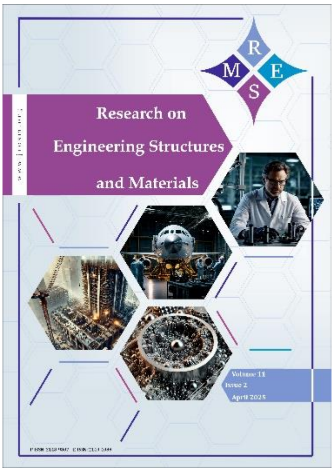

Thermal conductivity of functional fibrous inhomogeneous materials

Kriven Galina, Ryzhova Elizaveta

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Research Article

Thermal conductivity of functional fibrous inhomogeneous materials

Kriven Galina [*,a], Ryzhova Elizaveta [b]

Moscow Aviation Institute (National Research University), Russia

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Abstract

The study focuses on developing new methods for assessing the effective properties and modeling the thermal conductivity of fibrous composites with functional fibers for lightning protection systems on aircraft. The aim is to create more efficient and lightweight composites to enhance flight safety and reduce maintenance costs. The research methodology involves analyzing two types of whiskerized interphase layers in composites and modeling their thermal conductivity using a two-step homogenization procedure. The results indicate that composites with functional fibers can significantly outperform classical composites in terms of thermal conductivity. For composites where the whiskerized layer is formed by randomly grown and interwoven carbon nanotubes, the effective thermal conductivity in the plane perpendicular to the fiber axis and in the direction along the fiber can exceed those of classical composites by more than 2 and 1.2 times, respectively. For composites where the whiskerized layer consists of carbon nanotubes grown perpendicular to the fiber surface, these values can exceed those of classical composites by more than 3 and 1.1 times, respectively. Such findings suggest the potential use of functional composites as an effective replacement for metallic meshes in lightning protection systems on aircraft.

1. Introduction

Polymer composite materials (PCM) are widely used in aviation. Such materials are light in weight and have higher strength and stiffness values compared to materials such as aluminum, titanium and steel. For example, in the structures of Boeing 787 and Airbus A380 aircraft, the volume of PCM used in the structure reaches 50% by weight. However, polymer matrix composites are poor heat conductors, so non-conductive aircraft structures can be damaged by lightning strikes.

Lightning strikes can directly affect aircraft and sometimes cause sparks that pose a risk of igniting materials inside aircraft skins. A lightning bolt takes the path of least resistance. Therefore, if an aircraft is encountered on the way, it passes through its metal skin without penetrating inside and without touching important devices. To do this, the skin sheets must be tightly fitted to each other. In the case of using composite materials, it is necessary to apply additional technologies to protect against lightning, for example, the aircraft skin is covered with a layer of conductive copper foil mesh.

Efforts to enhance the thermal conductivity of carbon fiber and epoxy resin composites have been made in studies [1-3]. In study [4], zinc oxide particles hexagonally shaped and coated with boron nitride were introduced into the composite to increase conductivity. The thermal conductivity of such composite laminates increased by 78% and 90% at

*Corresponding author: kriven_galina@inbox.ru
[a] orcid.org/0000-0003-2340-2320; [b] orcid.org/0000-0002-3104-2743
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temperatures of 25°C and 100°C, respectively. In study [5] was shown that CNT/Al composite with a layered configuration exhibits the highest thermal conductivity. When the volume fraction of CNTs is approximately 3.7%, the CNT/Al composite demonstrates an outstanding effective thermal conductivity of 400 W/m·K, representing an increase of approximately 84% compared to that of the Al alloy.

In a number of works ([1-3]), it was shown that the addition of a small amount of carbon nanotubes (CNTs) leads to a disproportionate increase in the thermal conductivity of the composite. Thus, polymer composites can be converted into conductive materials, which increases their versatility. For example, in [1] it was found that adding 1% of single-walled carbon nanotubes (SWCNTs) of the total weight to epoxy resin leads to an increase in the thermal conductivity of the material by 125% at room temperature. In [2], an increase in thermal conductivity by 55% was measured for a composite containing 7% SWCNTs of the total weight of the polymer matrix. Authors of [3] reported a 57% increase in thermal conductivity with the addition of 7% multiwalled CNTs based on the total weight of the phenolic resin. The study [6] explores carbon nanotube (CNT) reinforced composites for honeycomb sandwich structures. Results show that adding CNTs up to 0.075 wt.% increases thermal stability and energy absorption.

Technologies for obtaining modern fibrous composites with special nanostructures (whiskers) grown on the surface are being actively developed at the present time. Such whiskers can be, for example, CNTs (fuzzy fibers) [7]. Since the improvement in the properties of composites depends on the characteristics of the whiskers grown on the fiber surface, the whiskerized fiber system is functional [8-11]. It has already been shown that it is possible to obtain a composite with simultaneously improved stiffness, strength, and damping proper-ties by modifying the CNT fiber surface [12-14]. Tests in [8] showed that the whiskerization of a fiber by CNTs leads to an increase in the interfacial strength of the composite material under longitudinal shear by 206% compared to the classical fibrous composite. Similar tests carried out in [9-10], showed an increase in the interfacial strength of whiskerized composites com-pared to classical composites by 175% and 150%, respectively. And authors of [11] conducted tests to determine the longitudinal and transverse compressive strengths, and showed that the longitudinal strength of the whiskerized composite increases by 43% compared to the classical composite, and the transverse strength, in turn, increases by 94%.

The dynamic properties of modified fibrous composites containing fibers with a whiskerized layer were first studied in works [15-17]. It was assumed that the fibers and the microstructure of the whiskerized layer are elastic, and the damping properties of the composite as a whole are related to the viscoelastic properties of the matrix. It was shown that the effective loss properties of the modified composite exceeded the loss modulus of the matrix by more than 20 times. Improved aircraft performance and reduced airframe weight can be achieved with new conductive modified composite materials with whiskerized fibers, since such materials combine high mechanical, thermal, electrical and physical proper-ties.

Two types of modified composites that differ in the orientation of whiskers in the interfacial layer are considered in the proposed work: 1) a modified compo-site, in which the whiskerized interfacial layer consists of randomly located and intertwined whiskers, 2) a modified composite in which the whiskers are grown perpendicular to the fiber surface. The purpose of the study is to simulate the effective thermal conductivity of modified composites with whiskerized fibers using a method based on a polydisperse model of a medium with spherical inclusions. The problems of determining the influence of the volume content of whiskers, the thickness of the interfacial layer and the volume content of the modified fiber on the effective thermal conductivity of the studied modified composites with whiskerized fibers are solved within the framework of the study. For the case when the interfacial layer is formed by whiskers grown perpendicular to the fiber surface, the effect of the whiskers radius and packing density (number of whiskers) on the effective thermal conductivity of the modified composite is estimated.

2. Study Description

Figure 1 shows the structure of the studied modified composite material with whiskerized fibers. The whiskerized interfacial layer is a nanocomposite that consists of whiskers and a matrix.

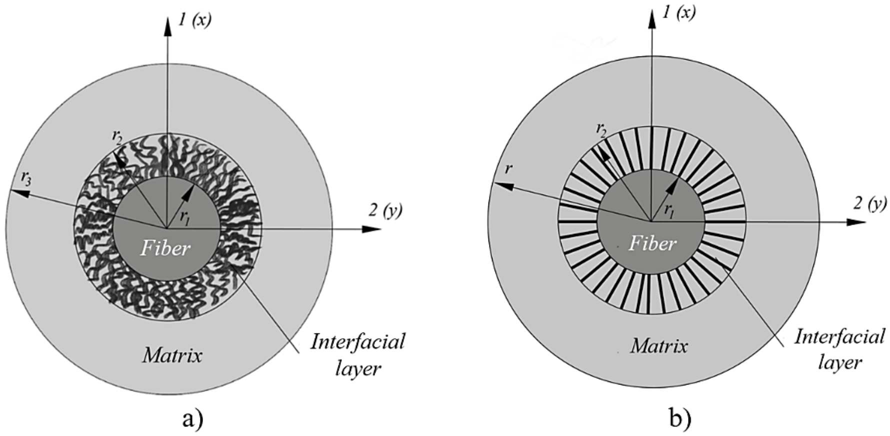


Fig. 1. Structure of modified composite material with whiskerized fibers: a) whiskers are arranged randomly and intertwined (case 1), b) whiskers are grown perpendicular to the fiber surface (case 2)

When modeling the effective thermal conductivity of such composites, we assume that the composite has a transversally isotropic structure with an isotropy plane across the fiber. Fiber and matrix are isotropic materials. In the case when the whiskers are randomly located in the interfacial layer and intertwined with each other (Fig. 1a), the whiskerized interfacial layer is also considered an isotropic material. And in the case when the whiskers are grown perpendicular to the surface of the base fiber (Fig. 1b), we consider that the whiskerized interfacial layer corresponds to a transversely isotropic material with an isotropy plane across the whiskers (case 2). Kriven, Shavelkin [18] study a fiber with a whiskered layer of CNTs grown randomly and intertwined. Carbon fiber with CNT whiskers grown perpendicular to the fiber surface was demonstrated in study [19].

The two-stage homogenization procedure is used to determine the effective thermal conductivity of the modified composite. At the first stage, the effective coefficient of thermal conductivity of the whiskerized layer is determined. The effective thermal conductivity coefficient of the whiskerized layer is determined using the polydisperse model of the medium in the case when it is assumed that the whiskerized layer is a macroscopically isotropic heterogeneous medium. And the effective thermal conductivity coefficient of the whiskerized layer is determined using a polydisperse model of a medium with cylindrical inclusions in the case when the whiskered layer is considered as a transversely isotropic material with an isotropy plane across the whiskers. When determining the effective thermal conductivity coefficient of such a composite, the volumetric content of whiskers in the interfacial layer is found taking into account all the geometric and physical parameters of the whiskers layer - the length of whiskers, their density, diameter, and thermal conductivity coefficient. After determining the effective thermal conductivity of the whiskerized interfacial layer, the effective thermal conductivity of the whiskered fibrous composite is found. For this, a polydisperse model of a medium with cylindrical inclusions, extended to a multiphase medium, is used.

A comparative evaluation of the effective thermal conductivity coefficients of modified composites with whiskerized fibers with the effective thermal conductivity coefficients of similar classical composites is carried out. The studied composites are formed by T-650 [20] carbon fiber and an epoxy matrix with thermal conductivity coefficients indicated in Table 1. In the modified composite, CNTs are grown on the surface of the carbon fiber. The influence of the volumetric content of inclusions (whiskers) on the effective thermal conductivity coefficient of the interfacial layer, as well as the influence of the thickness of the whiskerized layer, the volumetric content of whiskers and the volumetric content of modified fiber on the effective thermal conductivity of the entire composite is assessed. The volumetric content of whiskers in the interfacial layer and the volumetric content of modified fiber in the composite vary from 0 to 78%.

3. Effective Thermal Conductivity Coefficient Of The Studied Composite

The effective thermal conductivity of the modified whisker fiber composite is determined using a two-stage homogenization procedure. At the first stage, the effective coefficient of thermal conductivity of the whiskerized layer is determined.

In the case when the whiskerized layer is considered as an isotropic material, the effective thermal conductivity coefficient s determined by the well-known equation [21] for a three-phase model of a medium with spherical inclusions:

$$k_2^{(1)} = k_M \left(1 + \frac{C_0}{(1 - C_0)\ /\ 3 + k_M\ /\ k_1 - k_M)}\right) \tag{1}$$

where, $c_0 = a^3/b^3$: volume content of whiskers in the whiskerized interfacial layer, a: radius of the whiskers, b: radius of the shell from the matrix, k_1: thermal conductivity of the whiskers, k_m: thermal conductivity of the matrix.

In the case when the whiskerized layer is considered as a transversally isotropic material with the symmetry axis directed along the 1 axis, the Fourier heat conduction law can be written:

$$\begin{aligned} q_i{}^{(2)} &= -k_{ij}{}^{(2)} T_{,j}{}^{(2)} \\ q_i{}^{(2)} &= -k_{ij}{}^{(2)} \theta_{,j}{}^{(2)} \end{aligned} \tag{2}$$

where, q_i: heat flux vector in the whiskerized interfacial layer, $k_{ij}{}^{(2)}$: tensor of thermal conductivity coefficients in the whiskerized interfacial layer, $\theta_{,j}{}^{(2)}$: temperature in the whiskerized interfacial layer. In the last equation, only two components $k_{ij}{}^{(2)}$ are independent:

$$\begin{bmatrix} q_1^{(2)} \\ q_2^{(2)} \\ q_3^{(2)} \end{bmatrix} = \begin{bmatrix} -k_{11}{}^{(2)} & 0 & 0 \\ 0 & -k_{22}{}^{(2)} & 0 \\ 0 & 0 & -k_{33}{}^{(2)} \end{bmatrix} \begin{bmatrix} \theta_{,1}{}^{(2)} \\ \theta_{,2}{}^{(2)} \\ \theta_{,3}{}^{(2)} \end{bmatrix} \tag{3}$$

Then the effective thermal conductivity in the axial direction $k_{11}{}^{(2)}$ is determined by the mixture rule [4]:

$$k_{11}^{(1)} = \sum_{n=1}^{N} c_n k_n \tag{4}$$

where, N : number of phases with volume fractions c_n and thermal conductivity coefficients k_n. The effective thermal conductivity coefficient in the plane perpendicular to the whiskers axis $k_{33}^{(2)}$ is determined by the equation:

$$k_{33}^{(2)} = k_M\left(1+\frac{c_0^{(2)}}{(1-c_0^{(2)})/2+k_M/(k_I-k_M)}\right) \tag{5}$$

The volumetric content of whiskers in the whiskerized layer is determined by the equation:

$$c_0^{(2)} = \frac{M_b^2 d_b^2}{4\pi\left(l_b+D\right)D} \tag{6}$$

where, $c_0^{(2)}$: volume content of whiskers in the whiskerized interfacial layer in the case when the whiskers are grown perpendicular to the fiber surface, M_b : number of whiskers grown on the fiber surface, d_b : whiskers diameter, l_b : whiskers length, D : base fiber diameter. Taking into account the geometric features of the whisker layer, in which the whiskers are grown perpendicular to the fiber surface, it must be taken into account that the number of whiskers is limited:

$$M_b \le \pi D/d_b \tag{7}$$

At the second stage, the effective thermal conductivity of the entire composite is determined. In view of the transversal isotropy of the modified composite with the symmetry axis directed along the 3 axis, the Fourier heat conduction law can be written as:

$$\begin{aligned} q_i &= -k_{ij}T_{,j} \\ q_i &= -k_{ij}\theta_{,j} \end{aligned} \tag{8}$$

where, q_i : heat flux vector, k_{ij} : tensor of thermal conductivity coefficients, θ : temperature. Only two components k_{ij} are independent in the last equation:

$$\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} -k_{11} & 0 & 0 \\ 0 & -k_{11} & 0 \\ 0 & 0 & -k_{33} \end{bmatrix} \begin{bmatrix} \theta_{,1} \\ \theta_{,2} \\ \theta_{,3} \end{bmatrix} \tag{9}$$

The effective thermal conductivity in the axial direction k_{33}^{eff} is determined by the mixture rule:

$$k_{33}^{eff(i)} = \sum_{n=1}^{N} c_n k_n \tag{10}$$

where the index (i) corresponds to the considered case of the symmetry of the whiskerized interfacial layer. The following condition must be satisfied at infinity:

$$\theta\big|_{r\to\infty} \to \beta x_1 \tag{11}$$

where β is the temperature gradient. The stationary equations of heat conduction in the components of the composite have the form:

$$\begin{aligned} &\nabla^2\theta^1 = 0, && 0 \le r \le r_1, \\ &\nabla^2\theta^2 = 0, && r_1 \le r \le r_2, \\ &\nabla^2\theta^3 = 0, && r_2 \le r \le r_3, \\ &\nabla^2\theta^{eff} = 0, && r_3 \le r \le \infty, \end{aligned} \tag{12}$$

where θ^1, θ^2, θ^3, θ^{eff} are the temperatures in the fiber, the whiskerized interfacial layer, the matrix, and the effective medium, and ∇ is the Laplace operator. In a cylindrical coordinate system with axial symmetry with respect to x_3 we have:

$$\nabla = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \varphi^2} + \frac{\partial^2 u}{\partial z^2} \tag{13}$$

Then solution (12) with $r \to \infty, \theta_2(r,\theta) \to \beta r\cos\theta$ has the form:

$$\begin{aligned} &\theta^1 = A_1 r\cos\theta, && 0 \le r \le r_1, \\ &\theta^2 = (A_2 r + \frac{B_2}{r})\cos\theta, && r_1 \le r \le r_2, \\ &\theta^3 = (A_3 r + \frac{B_3}{r})\cos\theta, && r_2 \le r \le r_3, \\ &\theta^{eff} = (A_{eff} r + \frac{B_{eff}}{r})\cos\theta, && r_3 \le r \le \infty, \end{aligned} \tag{14}$$

It is assumed that a uniform field is realized at infinity, which corresponds to $B_{eff} = 0$ with a unit heat flux $A_{eff} = 1$ [21-22]. To write the boundary conditions, we assume that the heat fluxes are also continuous at the phase boundary. Six unknowns, including the effective thermal conductivity k_{eff}, are determined from a system of six equations:

$$\begin{aligned} &1)\ \theta^I - \theta^2 = 0, && r = r_1, \\ &2)\ \theta^2 - \theta^3 = 0, && r = r_2, \\ &3)\ \theta^3 - \theta^{eff} = 0, && r = r_3, \\ &4)\ -k_1\frac{\partial\theta^1}{\partial r} + k_2^{(i)}\frac{\partial\theta^2}{\partial r} = 0, && r = r_1, \\ &5)\ -k_2^{(i)}\frac{\partial\theta^2}{\partial r} + k_3\frac{\partial\theta^3}{\partial r} = 0, && r = r_2, \\ &6)\ -k_3\frac{\partial\theta^3}{\partial r} + k_{11}^{eff(i)}\frac{\partial\theta^{eff}}{\partial r} = 0, && r = r_3, \end{aligned} \tag{15}$$

Thus, in the case of a whiskerized interfacial layer with isotropic properties $k_2^{(i)} = k_2^{(1)}$ (1), and in the case of a whiskerized interfacial layer with transversally isotropic properties $k_2^{(i)} = k_{33}^{(2)}$ (4).

The solution of the system of equations (15) taking into account (14) with respect to $k_{11}^{eff(i)}$ has the form:

$$k_{11}^{eff(i)} = -k_3 \left(2 - \frac{3}{1 + D / (k_1 k_3 m - k_1 k_2^{(i)} n + (k_2^{(i)})^2 m - k_2^{(i)} k_3 n)} \right) \quad (16)$$

where $m = (-2 + l)l$, $n = 2 + (-2 + l)l$, $l = r_2 - r_1$ is the thickness of the interfacial layer, $D = k_1 k_3 c_{vol} a + k_1 k_2^{(i)} c_{vol} b - (k_2^{(i)})^2 c_{vol} a - c_{vol} k_2^{(i)} k_3 b$. Thus, the effective thermal conductivity coefficients of the whiskered layer ($k_2^{(1)}, k_{11}^{(2)}, k_{33}^{(2)}$) and the modified composite with whiskered fibers in the direction along the fiber $k_{33}^{eff(i)}$ and in the plane perpendicular to the fiber axis $k_{11}^{eff(i)}$ are determined.

4. Results and Discussion

The effective thermal conductivity of the modified composite with whiskerized fibers was determined using a two-stage homogenization procedure. In the first stage, the effective properties of the whiskerized interfacial layer were determined.

This study investigated the influence of the volume content of inclusions (whiskers) on the effective thermal conductivity of the interfacial layer formed by grown CNTs in two versions. The first variant of the interfacial layer is formed by randomly grown, intertwined CNTs, considered as an isotropic material. The second variant of the interfacial layer is formed by CNTs grown perpendicular to the fiber surface, considered as a transversely isotropic material. The properties of the structural elements of the interfacial layer are shown in Table 1.

Table 1. Physical properties of structural elements of a modified composite with whiskerized fibers [20, 23.24]

	Carbon fiber T-650	CNT	Epoxy Matrix
Thermal conductivity coefficient (W/(m·K))	14	3000	0.195-0.255

The effective thermal conductivity of the interfacial layer, considered as an isotropic material, was determined by equation (1). The effective thermal conductivity coefficients of the interfacial layer, considered as a transversally isotropic material, were determined by equations (4) and (5).

The effective thermal conductivity coefficient of the interfacial whiskerized layer in the plane perpendicular to the fiber surface (case 2), as the volume content of the inclusion increases, grows commensurately with the increase in the effective thermal conductivity coefficient of the interfacial whiskerized layer, considered as an isotropic material (case 1) (Figure 3). And the effective thermal conductivity of the interfacial whiskerized layer in the direction along the whiskers (case 2) rapidly increases with the increase in the volume content of CNTs (Figure 4) - more than 12,000 times compared to the thermal conductivity of the matrix. However, in the direction across the whiskers, the whiskerized layer formed by interwoven whiskers allows achieving an effective thermal conductivity exceeding that in the whiskerized layer formed by whiskers grown perpendicular to the fiber by more than 1.5 times. But in the direction along the whiskers, in the case where whiskers intertwine, the effective properties of the whiskerized layer (case 1) remain the same as in the direction across the whiskers, while the properties of the whiskerized layer formed by whiskers grown perpendicular to the fiber (case 2) increase by more than 1000 times compared to the effective properties of the whiskerized layer formed by interwoven whiskers (case 1). The effective thermal conductivity of the whiskerized layer with a low volume fraction (up to 2.5%) of randomly oriented and interwoven whiskers (case 1) is approximately 0.2-0.3 W/(m·K), which corresponds to the experimental results obtained in [4].

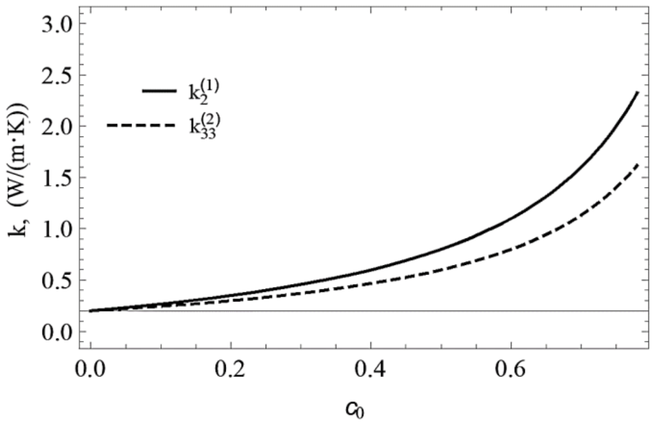


Fig. 2. Dependence of the effective thermal conductivity coefficient (in the direction along the fiber axis) on the volume content of CNTs in the interfacial layer

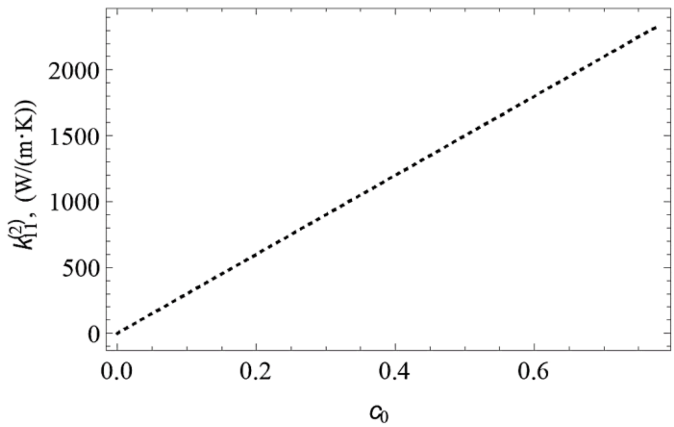
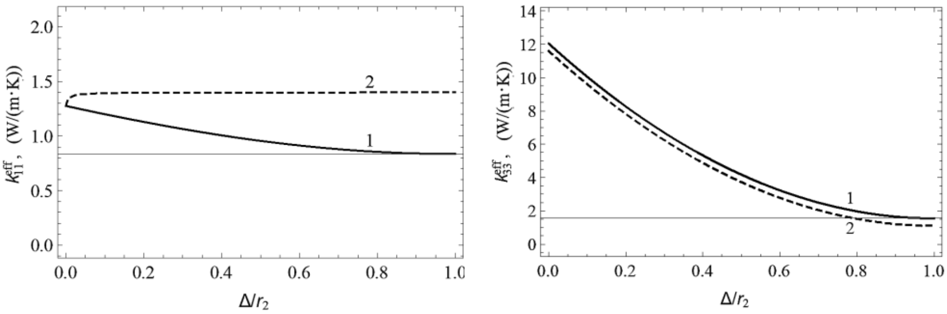


Fig. 3. Dependence of the effective coefficient of thermal conductivity in the direction along the CNT of a transversally isotropic layer on the volume content of CNTs in the interfacial layer

The effective thermal conductivity coefficient for a modified composite with whiskerized fibers, consisting of T-650 carbon fiber, CNTs, and an epoxy matrix, has been studied. The properties of the structural elements of such a composite are shown in Table 1. For the cases where the whiskerized layer is a macroscopically isotropic heterogeneous medium and when the whiskered layer is a transversely isotropic medium, the effective thermal conductivity coefficient in the plane perpendicular to the fiber axis was obtained using equation (16), and the effective thermal conductivity coefficient in the direction along the fiber axis was obtained from equation (10).

It is necessary to evaluate the effect of the thickness of the whiskerized layer on the effective thermal conductivity of the composites under consideration. For this, we consider a composite with a constant modified fiber radius $r_2 = 1$, the thickness of the whiskerized interfacial layer Δ / r_2, and the matrix radius r_3 depending on the volume content of the modified fiber $r_3 = r_2 / \sqrt{c_{vol}}$ at $c_{vol} = 78\%$ and $c_0 = 78\%$ characteristic of the most dense packing of inclusions in a square periodic structure. Figure 5 shows the plots of effective thermal conductivity coefficients in the plane perpendicular to the fiber axis $k_{11}^{eff(i)}$ and in the direction along the fiber axis $k_{33}^{eff(i)}$ on the thickness of the whiskerized layer Δ / r_2.



(a) (b)

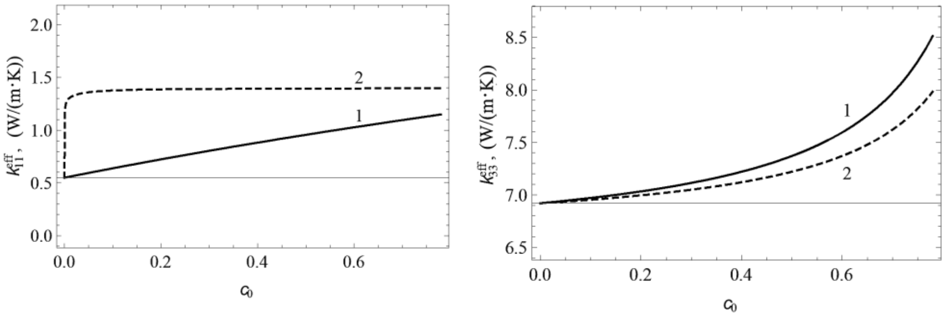
Fig. 4. Graphs of dependences of effective thermal conductivity coefficients on the thickness of the whiskered layer: a) $k_{11}^{eff(i)}$ - in the plane perpendicular to the fiber axis, b) $k_{33}^{eff(i)}$ - in the direction along the fiber axis

In Figure 5 and all subsequent figures, the graph corresponding to the case when the whiskerized interfacial layer is an isotropic medium is indicated by the number 1, and the graph corresponding to the case when the whiskerized interfacial layer is a transversely isotropic medium is indicated by the number 2.

Figure 5a illustrates that the effective thermal conductivity in the plane perpendicular to the fiber surface remains practically unchanged for the case when the whisker layer is a transversely isotropic medium, regardless of the thickness of the whisker layer. However, for the case when the whisker layer is an isotropic medium, there is a slight decrease in the thermal conductivity coefficient as the thickness of the whisker layer increases. In Figure 5b, the decrease in the effective thermal conductivity in the direction along the fiber is shown as the thickness of the whisker layer increases for both considered cases.

Since the study involved a fixed radius of modified fibers, the decrease in the effective thermal conductivity is associated with the replacement of fibers by a whiskerized layer with a low thermal conductivity matrix. The effect of reducing the effective thermal conductivity is observed only in case 2 in the plane perpendicular to the fiber axis because in such a composite, the effective properties of the whiskerized layer in the direction across the fiber axis (along the whisker axis) significantly exceed the properties of the carbon fiber (Figures 2 and 3), and there is no substitution of a high thermal conductivity layer with a low thermal conductivity layer. From the perspective of achieving stable high values of the effective thermal conductivity in both considered directions, case 2 is preferred, where short fibers are grown perpendicular to the fiber surface.

The influence of the volume content of whiskers on the effective thermal conductivity of the modified composite is shown in Figure 6. When plotting graphs (Figure 6), the fixed values were the thickness of the whiskerized layer ($0,2\Delta / r_2$) and the volume content of the modified fiber c_{vol}= 75%.

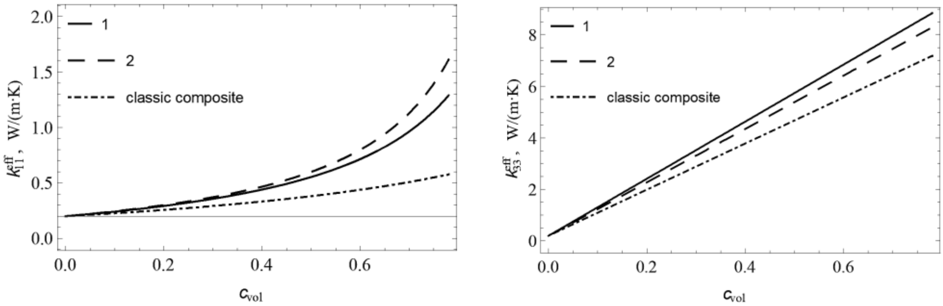


(a) (b)

Fig. 5. Graphs of dependences of effective thermal conductivity coefficients on the volume content of CNTs in the whiskerized interfacial layer: a) $k_{11}^{eff(i)}$ - in the plane perpendicular to the fiber axis, b) $k_{33}^{eff(i)}$ - in the direction along the fiber axis

Figure 6a shows that even with a slight increase in the volume content of whiskers in the interfacial layer of the composite with CNTs grown perpendicular to the fiber surface, the effective thermal conductivity coefficient in the plane perpendicular to the fiber axis is more than 2 times higher than the thermal conductivity coefficient of the classical composite (the value on the graph at $c_0 = 78\%$) with the same volumetric fiber content ($c_{vol} = 78\%$). At the same time, these properties remain stable with a further increase in the volume content of CNTs in the interfacial layer. In the direction along the fiber, the composite with CNTs grown randomly and intertwined with each other demonstrates slightly higher effective thermal conductivity than the composite with CNTs grown perpendicular to the fiber surface (Figure 6b). The effective thermal conductivity simultaneously takes the highest values in both considered directions with the maximum volume fraction of whiskers in the whiskerized interphase layer. However, in the plane perpendicular to the fiber axis, the effective thermal conductivity for case 2 exceeds that for case 1 by more than 1.2 times, while in the direction along the fiber axis, the effective thermal conductivity for case 1 exceeds that for case 2 by more than 1.06 times. This is because in the direction along the fiber axis, which corresponds to the direction across the whisker axis, the properties of the whiskerized layer formed by both whiskers grown perpendicular to the fiber and randomly grown whiskers differ, but not as significantly as in the direction perpendicular to the fiber axis, which corresponds to the direction along the whisker axis (Figures 2 and 3). Therefore, the optimal structure of the modified composite with whiskerized fibers can be considered as the composite with the maximum possible volume fraction of whiskers grown perpendicular to the fiber (case 2).

When constructing graphs (Figure 7), the volume content of CNTs in the interfacial layer was a fixed value equal to $c_0 = 70\%$ and the length of the whiskers was also a fixed value equal to $0,2\Delta / r_2$. Figure 7 also plots the dependence of the effective coefficient on the volumetric fiber content in the classical composite.



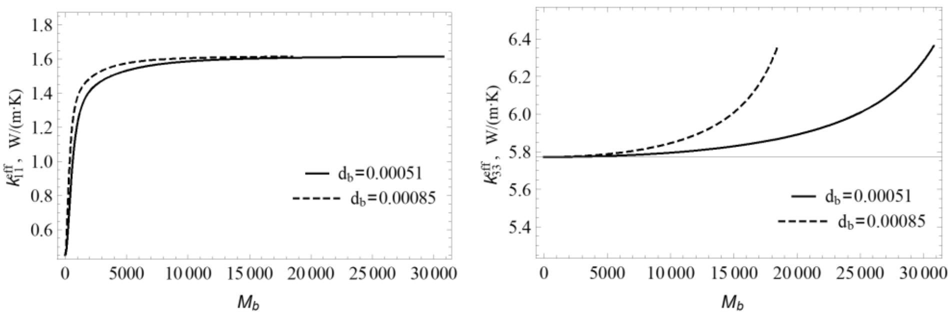
(a) (b)

Fig. 6. Graphs of dependences of effective thermal conductivity coefficients on the volume content of the modified fiber: a) $k_{11}^{eff(i)}$ - in the plane perpendicular to the fiber axis, b) $k_{33}^{eff(i)}$ - in the direction along the fiber axis

It can be seen (Figure 7) that at the maximum volume content of the modified fiber $c_{vol} = 78\%$ it is possible to achieve a significant increase in the effective thermal conductivity coefficients in the plane perpendicular to the fiber axis compared to the effective thermal conductivity coefficients of similar classical composites (more than 2 times for case 1 and more than 3 times for case 2). In such composites, the matrix layer with a low thermal conductivity is practically absent, and the role of the binder is performed by the whiskerized layer, the effective thermal conductivity properties of which depend on how this whiskerized layer is formed. In the plane perpendicular to the fiber axis, the effective thermal conductivity for case 2 exceeds that for case 1 by more than 1.2 times, while in the direction along the fiber axis, the effective thermal conductivity for case 1 exceeds that for case 2 by more than 1.01 times. Therefore, the optimal structure of the modified composite with whiskerized fibers can be considered as a composite with the maximum volume fraction of modified fibers, in which the modification is carried out by growing whiskers perpendicular to the fiber surface (case 2).

Let us consider a specific example of a modified composite consisting of a 5 μm diameter carbon fiber and carbon nanotubes grown perpendicular to the fiber surface. The geometric parameters include whisker lengths ranging from 1 to 2 μm and whisker diameters ranging from 0.00051 to 0.00085 μm [19], [23]. The physical properties of the composite under study are provided in Table 1. According to equation (7), with a whiskers diameter of 0.00051 μm, the maximum number of whiskers grown perpendicular to the fiber surface is 30 799, and with a whiskers diameter of 0.00085 μm, the maximum number of whiskers is 18,480. With a whiskers length of 1 μm, this is corresponding to the volumetric content of whiskers in the interfacial layer 65%, and with a whiskers length of 2 μm - 56% (eq. 6). It has already been shown (Figure 4) that an increase in the length of the whiskers (thickness of the whisker layer) negatively affects the effective thermal conductivity in the direction along the fiber. It has also been shown that an increase in the volume content of the modified fiber is accompanied by an increase in the effective thermal conductivity in all directions (Figure 7). Therefore, having fixed the minimum possible CNT length equal to 1 μm and the maximum possible volume content of the modified fiber $c_{vol} = 78\%$, we estimate the effect of the number of whiskers on the effective thermal conductivity of the composite under study.

Figure 8 shows the dependences of the effective thermal conductivity coefficients on the number of whiskers associated with the whiskers diameters. It can be seen (Figure 8 a) that the effective thermal conductivity in the plane perpendicular to the fiber axis grows rapidly as the number of whiskers increases, but when the number of whiskers reaches a certain value (in this case, 5000 whiskers), the effective thermal conductivity in the plane perpendicular to the fiber axis remains practically unchanged at further increase in the number of whiskers. Also, the effective thermal conductivity in the plane perpendicular to the fiber axis is not significantly affected by the whiskers diameter. And in the direction along the fiber axis (Figure 7b), the following trend is observed: an increase in the thermal conductivity coefficient is achieved only with simultaneous increases in the number and diameter of the whiskers, as only in this case can a dense packing of whiskers with a high thermal conductivity coefficient be obtained. Otherwise, the space between the whiskers in the whiskerized layer is occupied by a matrix with a low thermal conductivity coefficient, which leads to a decrease in the effective thermal conductivity of the whiskerized interphase layer in the direction perpendicular to the whiskers, and consequently, to a decrease in the effective thermal conductivity of the entire composite in the direction along the fiber axis. Therefore, if it is important to maintain high values of the effective thermal conductivity coefficient in the direction along the fiber axis, it is necessary to select the number of whiskers taking into account their diameter so that the volume fraction of whiskers in the whiskerized layer is maximum (Equation 7).



(a) (b)

Fig. 7. Graphs of dependences of effective thermal conductivity coefficients on the number of CNTs in a whiskerized interfacial layer, in the case when whiskers are grown perpendicular to the fiber surface: a) $k_{11}^{eff(i)}$ - in the plane perpendicular to the fiber axis, b) $k_{33}^{eff(i)}$ - in the direction along the fiber axis

Thus, modified composites with whiskers grown perpendicular to the fiber surface are preferable to modified composites with whiskers grown randomly and intertwined with each other from the perspective of increasing the effective thermal conductivity in the plane perpendicular to the fiber axis. The effective coefficient of thermal conductivity in the direction along the fiber axis is insignificant but higher for modified composites with whiskers grown randomly and intertwined with each other. Despite this, it is difficult to control the volume content of whiskers that are randomly located and intertwined with each other, and in fact, the interfacial layer consisting of such whiskers and a matrix has anisotropic properties. Therefore, to ensure the planned thermal conductivity coefficients, it is preferable to use modified composites with whiskers grown perpendicular to the fiber surface. Growing CNTs perpendicular to the fiber surface makes it possible to control the effective thermal conductivity in various directions and in a wide range by changing the thickness of the whisker layer, the volume content of the modified fiber, and the volume content of whiskers, which depends on the length of the interfacial layer, the diameter of the whiskers, and the number of whiskers.

5. Conclusion

In this research study, an analysis of the effective thermal conductivity of modified composites with whiskerized fibers was conducted. The impact of various parameters such as the thickness of the whiskerized interphase layer, volume fraction of whiskers, number, and diameter of whiskers on the thermal conductivity of the composite in different directions was investigated. To achieve this, a polydisperse medium model with spherical inclusions, as proposed by Hashin and Shtrikman, was used to determine the effective thermal conductivity coefficient of the composite with whiskerized fibers. The obtained results were analyzed to identify the optimal structure of the composite with the maximum effective thermal conductivity coefficient.

The study revealed that the effective thermal conductivity coefficient of modified composites with whiskerized fibers can be significantly increased by increasing the thickness of the whiskerized interphase layer. For instance, when the thickness of the whiskerized layer increases from 1 μm to 2 μm, the effective thermal conductivity coefficient in the direction along the fiber can increase by more than 1.2 times. It was found that the optimal structure of modified composites with whiskerized fibers is those with the maximum possible volume fraction of whiskers, grown perpendicular to the fiber surface. Such composites provide a high effective thermal conductivity coefficient both in the plane perpendicular to the fiber axis and in the direction along the fiber axis. The effective thermal conductivity coefficient of modified composites with whiskerized fibers increases depending on the increase in the volume fraction of whiskers in the interphase layer. For example, when the volume fraction of whiskers increases from 30% to 65% in the plane perpendicular to the fiber axis (case 2), the effective thermal conductivity coefficient can increase by more than 2 times.

Analysis showed that increasing the volume fraction of modified fibers also contributes to the increase in the effective thermal conductivity coefficient. For instance, with the maximum volume fraction of modified fibers (volume fraction of whiskers in the interphase layer being 65%), the effective thermal conductivity coefficient in the plane perpendicular to the fiber axis can increase by more than 3 times compared to classical composites. A numerical analysis was conducted to investigate the influence of the number of whiskers on the effective thermal conductivity coefficient. The dependency graphs of effective thermal conductivity coefficients on the number of whiskers show that in the plane perpendicular to the fiber axis, the effective thermal conductivity coefficient rapidly increases with the increase in the number of whiskers and reaches an almost constant value after a certain value (for example, around 5000 whiskers).

As a result of analyzing the influence of whisker diameter and their number on the effective thermal conductivity coefficient, it was revealed that the optimal value of the effective thermal conductivity coefficient is achieved with a certain combination of whisker number and diameter. This highlights the necessity of careful control over these parameters when designing modified composites with whiskerized fibers.

Our studies also confirmed that modified composites with whiskerized fibers, grown perpendicular to the fiber surface, are preferable compared to composites where whiskers are grown randomly and intertwined. This preference is due to higher values of the effective thermal conductivity coefficient in the plane perpendicular to the fiber axis.

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