Porosity influence of power generating equipment structural materials on its thermoelastic characteristics and thermal conductivity

V.S. Zarubin¹, E.S. Sergeeva²

¹Bauman Moscow State Technical University, 2-nd Baumanskaya, 5, Moscow, 105005, Russia
²JSC "Kompozit", Pionerskaya, 4, Korolev, Moscow Region, 141070, Russia
E-mail: sergeeva.e.s@outlook.com

Abstract. This paper outlines simulation models that represent the quantitative interdependencies between the thermal conductivity and the thermoelastic properties of composites, on the one hand, and their porous structure and matrix properties, as well as the volume fraction of their reinforcing inclusions, on the other hand. As the reinforcing inclusions, randomly-oriented anisotropic single-wall carbon nanotubes (SWNT) are taken. The key means for constructing the simulation models are the self-matching method and the dual variational formulation of the thermal conductivity/thermoelasticity problem for a non-homogeneous solid body. With the simulation models presented below, it is possible to estimate the effect the nanocomposite porosity has on the thermoelastic properties and thermal conductivity of nanocomposites.

1. Introduction
A composite represents a basic material (matrix), prevailing by volume, modified with a non-homogeneous structure in the form of a system of separate inclusions. The composites are extensively used as a material for heat-stressed structural components designed to operate under severe concurrent mechanical and thermal loads. The actual area of application of the composites depends largely on their thermoelastic and thermophysical characteristics such as the elasticity modulus, the thermal coefficient of linear expansion (CLE) and the thermal conductivity coefficient.

The most widely used types of the composite matrix are polymeric and metal ones, given the specific requirements to the matrix processing behavior. However, the composite manufacturing process is rarely optimized so as to avoid occurrence of material defects such as porosity.

As a reinforcing agent, inclusions of various nature and shapes are used [1, 2, 3, 4, 5, 6]. Lately, nanostructural objects (fullerenes, graphene flakes, single-wall carbon nanotubes, nanoscale clusters) [7, 8, 9] are considered as reinforcing agents for material strengthening. Even with a small proportion of these objects, the elastic properties can be enhanced significantly [10].

This paper discusses a porous nanocomposite reinforced with randomly-oriented single-wall carbon nanotubes. There are plenty of publications addressing the elastic properties of this material; however, the effect of the composite porous structure on its thermoelastic properties and thermal conductivity has been studied in lesser detail.
2. Basic relations

Let us consider a porous composite reinforced with randomly-oriented single-wall carbon nanotubes in the form of an elongated ellipsoid of rotation. The elastic properties of a single-wall carbon nanotube can be described with tensor $C^\bullet$. The tensor components are associated with the graphene elastic moduli via the matrix corresponding to tensor $S^\bullet$ through the following relations [11]:

\[
S_{11} = \frac{1 - \eta}{4\eta E_g} + \frac{1/16}{G_g(1 - \eta)^2\eta}, \quad S_{12} = \frac{1 - \eta}{4\eta E_g} - \frac{1/16}{G_g(1 - \eta)^2\eta}, \quad S_{13} = \frac{-\nu_g/4}{\eta(1 - \eta)E_g},
\]

\[
S_{33} = \frac{1/4}{\eta(1 - \eta)E_g}, \quad S_{44} = \frac{1}{2(1 - \eta)G_g},
\]

where $C^\bullet$ — fourth-order tensor of the single-wall carbon nanotube elasticity coefficients; $S^\bullet$ — fourth-order tensor of the single-wall carbon nanotube compliance coefficients; $E_g$ — Young’s modulus of graphene, Pa; $\nu_g$ — Poisson’s ratio of graphene; $G_g$ — shear modulus of graphene, GPa; $\eta = h/D = h/\sqrt{3}d_0\sqrt{m^2 + n^2 + mn}/\pi$; $h = 0.075$ — apparent thickness of single-layer graphene, nm; $D$ — single-wall carbon nanotube diameter, nm; $(m,n)$ — single-wall carbon nanotube chirality indices; $d_0 = 0.142$ — distance between two neighboring atoms of carbon in the graphene plane, nm.

In terms of thermal expansion, a single-wall carbon nanotube can be considered isotropic [12]. The inclusions are assumed to be randomly arranged, which makes it possible to consider the composite as macroscopically isotropic. This being the case, the elastic properties of the composite can be fully described with the following relation:

\[
C = 3KV + 2GD,
\]

where $K$ — volumetric elasticity modulus of the composite, GPa; $G$ — shear modulus of the composite, GPa; $V$ — volumetric part of $I$; $D$ — deviatoric part of $I$; $I$ — fourth-order unit tensor.

The composite matrix is considered isotropic and its elastic properties are fully described using an isotropic fourth-order tensor:

\[
C^\circ = 3K^\circ V + 2G^\circ D,
\]

where $C^\circ$ — fourth-order tensor of matrix material elasticity coefficients; $K^\circ$ — volumetric elasticity modulus of the composite, GPa; $G^\circ$ — shear modulus of the matrix, GPa.

The composite matrix is also considered isotropic in terms of thermal expansion.

The thermoelastic properties of the pores can be described using tensors $C^\prime$ — fourth-order tensor of pores elasticity coefficients, its components being zero, and $\alpha^\prime$ — second-order tensor of temperature deformation coefficients having components $\alpha^\prime\delta_{ij}$, with their components having zero values.

3. Simulation models

The simulation models are built using the self-consistent method [13, 14], and for a non-porous composite — using the dual variation formulation of the thermal conductivity / thermoelasticity problem for a non-homogenous solid body [15].

3.1. Thermoelastic module

To estimate the thermoelastic moduli of a porous nanocomposite, the self-consistent method [13, 14] is used. The method is applied twice: first, to determine the elastic moduli, and then, to
find TCLE. With this method, the main relationships for modules $K$ and $G$ of the material under study are as follows:

$$C_V u_1^* + (1 - C_V - C'_V) u_1^0 + C'_V u_1'\quad C_V u_2^* + (1 - C_V - C'_V) u_2^0 + C'_V u_2'.$$

(3)

Here

$$u_1^* = u^* \cdots V, \quad u_2^* = u^* \cdots D,$$

$$u_1^0 = u^0 \cdots V, \quad u_2^0 = u^0 \cdots D,$$

$$u_1' = u' \cdots V, \quad u_2' = u' \cdots D,$$

$$u^* = (C^* - C + C \cdot W^*)^{-1} \cdots (C - C^*),$$

$$u^0 = (C^0 - C + C \cdot W)^{-1} \cdots (C - C^0),$$

$$u' = (C' - C + C \cdot W)^{-1} \cdots (C - C'),$$

$$C \cdot W = (3K + 4G) V + 5/3 ((3K + 4G) / (K + 2G) D),$$

where $W$ — isotropic Eshelby’s tensor.

Tensor $W^*$ corresponds to a square matrix of the sixth order having seven independent elements [14, 16]:

$$N_{11} = N_{22} = Q D_{11} + R D_1, \quad N_{12} = N_{21} = Q D_{11}/3 - R D_1,$$

$$N_{33} = Q D_{33} + R D_3, \quad N_{31} = N_{32} = b^2 Q D_{11} - R D_3,$$

$$N_{13} = N_{23} = Q D_{13} - R D_1, \quad N_{66} = Q D_{11}/3 + R D_1,$$

$$N_{44} = N_{55} = Q (1 + b^2) N_{13}/2 + R (1 - D_1)/2,$$

where

$$D_1 = \frac{b (b (1 - b^2)^{1/2} - \text{arccosh} b)}{2 (1 - b^2)^{3/2}}, \quad D_3 = 1 - 2 D_1,$$

$$D_{11} = \frac{1 - 3 D_{13} b^2}{4}, \quad D_{13} = (D_1 - D_3) / (3 (1 - b^2)), \quad D_{33} = 1/3 - 2 D_{13}.$$

Here $b$ — ratio of minor to major semi-axes of the ellipsoid; $Q = 3/2 (1 - \nu)$, $R = (1/2 - \nu) / (1 - \nu)$. The rest of the matrix elements are zero.

After calculating the elasticity moduli of the composite, the result of averaging the perturbations of the strained state of the inclusions, matrix particles and pores throughout the representative volume of the composite can be represented as the following equation:

$$C_V \langle v^* \rangle + (1 - C_V - C'_V) \langle v^0 \rangle + C'_V \langle v' \rangle = O_2$$

(4)

that comprises second-order tensors:

$$v^* = (C^* - C + C \cdot W^*)^{-1} \cdots (C - C^*) \cdots (\alpha^* - \alpha),$$

$$v^0 = (C^0 - C + C \cdot W)^{-1} \cdots (C - C^0) \cdots (\alpha^0 - \alpha),$$

$$v' = (C' - C + C \cdot W)^{-1} \cdots (C - C') \cdots (\alpha' - \alpha).$$

Here $C_V$ — total proportion of reinforcing inclusions, %; $C'_V$ — volumetric porosity of the composite, %; $\alpha^*$ — TCLE of graphene in the plane of isotropy; $\alpha^0$ — second-order tensor of matrix material temperature deformation coefficients having components $\alpha^0 \delta_{ij}$.

Averaging of these tensors amounts to calculation of their first invariants by contraction with second-order unit tensor $I_2$. As a result, for equation (4) we have

$$C_V v^* \cdot I_2 + (1 - C_V - C'_V) v^0 \cdot I_2 + C'_V v' \cdot I_2 = 0$$

in terms of the thermal coefficient of linear expansion $\alpha$ of interest.
3.2. Thermal conductivity

To determine the thermal conductivity coefficient, the simulation model of heat transfer [17] in a porous composite reinforced with single-wall carbon nanotubes involves two steps, the first one considering interaction between an isotropic matrix and spherical particles representing the pores, while the second one considering interaction between an isotropic porous matrix with elongated ellipsoids of rotation.

From consideration of the thermal interaction between the matrix particles and the pores, we have the following relationship that can be used to determine the porous matrix thermal conductivity coefficient:

\[ \tilde{\lambda}^o = \lambda^o \frac{1 + (\bar{\lambda} - 1) \left( \frac{1}{3} (1 + 2C'_V) \right)}{1 + (\bar{\lambda} - 1) \frac{1}{3} (1 - C'_V) }, \quad \bar{\lambda} = \lambda' \frac{\lambda^o}{\bar{\lambda}} . \]

Here \( \lambda^o \) — matrix material thermal conductivity coefficient, W/(m·K); \( \lambda' \) — pore thermal conductivity coefficient, W/(m·K); \( \tilde{\lambda}^o \) — porous matrix thermal conductivity coefficient, W/(m·K); \( \lambda \) — composite thermal conductivity coefficient.

Considering the thermal interaction between a certain single-wall carbon nanotube and its surrounding unlimited volume of the matrix, followed by volume-wise averaging of the composite characteristics, we come to the following relationship for determining the thermal conductivity coefficient of the composite with a porous matrix reinforced with ellipsoidal inclusions:

\[ \lambda = \frac{\tilde{\lambda}_a}{3}, \]

where

\[ \tilde{\lambda}_a = \frac{1 + (\bar{\lambda}' - 1) (D_a + (1 - D_a) C_V)}{1 + (\bar{\lambda}' - 1) D_a (1 - C_V) }, \quad \bar{\lambda}' = \lambda' \frac{\lambda^o}{\bar{\lambda}}, \quad \alpha = 1, 2, 3, \]

\[ D_1 = D_2 = \left( 1 - b^2 \ln (2/b) \right) / 2, \quad D_3 = b^2 (\ln (2/b) - 1) . \]

4. Results of mathematical modeling

As the initial data for the graphene thermoelastic properties, the following values were taken:

\[ E_g = 1.1 \text{ TPa}, \quad \nu_g = 0.412 \text{ [18]}, \quad \alpha_g = 0.7 \cdot 10^{-6} \text{ K}^{-1} \text{ [11]}. \]

For the modeling, zigzag-type single-wall carbon nanotubes, their chirality index being (10, 10), represented by an elongated ellipsoid of rotation with ellipticity (minor to major semiaxes ratio) \( b = 0.01 \), were chosen.

Quantitative analysis of the dependence of the composite thermoelastic characteristics on the input parameters of the matrix, the reinforcing members, as well as the material composition, is performed for a composite with an aluminum matrix, for which the following values are taken:

\[ K^o = 76.3 \text{ GPa}, \quad G^o = 25.5 \text{ GPa} \text{ [1]}, \quad \lambda^o = 250.0 \text{ W}/(\text{m} \cdot \text{K}) \text{ [19]}, \quad \alpha^o = 23.3 \cdot 10^{-6} \text{ K}^{-1} \text{ [12]}. \]

For a single-wall carbon nanotube, the following values are chosen:

\[ \lambda_1^* = \lambda_2^* = 875.0 \text{ W}/(\text{m} \cdot \text{K}), \quad \lambda_3^* = 691.0 \text{ W}/(\text{m} \cdot \text{K}) \text{ [20]}. \]

Here \( \lambda_1^* = \lambda_2^* \) — effective thermal conductivity coefficient of a single-wall carbon nanotube normal to the longitudinal axis, W/(m·K); \( \lambda_3^* \) — effective thermal conductivity coefficient of a single-wall carbon nanotube along the longitudinal axis, W/(m·K).
Figures 1, 2, and 3 show the elastic moduli, TCLE and the thermal conductivity coefficient, correspondingly, versus porosity $C_V'$ and parameter $\tilde{C}_V = C_V / (1 - C_V')$, obtained for a composite reinforced with randomly-oriented single-wall carbon nanotubes.

It can be seen that the elastic characteristics of the composite deteriorate significantly with $C_V' = 0.4$, while its TCLE and thermal conductivity coefficient are less sensitive to porosity variations.
5. Conclusion
The mathematical model representing the thermoelastic and thermal interaction between an anisotropic ellipsoidal inclusion and an isotropic medium made it possible to estimate the thermoelastic properties and the thermal conductivity coefficient of the composite reinforced with randomly-oriented single-wall carbon nanotubes, as well as the isotropic matrix, with due account for the porosity. The elastic characteristics of the composite were found to show much stronger dependence on the material porosity, as against the dependence on the thermal conductivity coefficient and TCLE. With the relationships given above, it is possible to predict the thermoelastic parameters and the thermal conductivity coefficient of a porous composite based on the specified characteristics, the volume proportion of the reinforcing ellipsoidal inclusions, as well as the matrix properties.

5.1. Acknowledgments
The work was performed within the framework of implementation of the basic part of the governmental task of the Ministry of Education and Science of the Russian Federation (Project 9.7784.2017/BP).

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