Thermal Conductivity Structure and Anisotropy of the Colossal Carbon Mesotubes

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Abstract. A model of a tube with a square cross-section was compiled for the mathematical analysis of the mesotube in Cartesian coordinates, with the selection of an element of a representative volume. To estimate the effective thermal conductivity of the structure, the generalized theory of conductivity with linearization of heat flux streamlines was used. The presence of anisotropy leads to the division of the problem into a separate estimate of the longitudinal and transverse thermal conductivity. The cross-section of the model was divided into elementary sections by a system of auxiliary adiabatic and isothermal planes, then the sections of the model were presented in the form of thermal resistances connected in chains - electrical circuits. Using the analogy of the identity of thermal and electrical resistances, the total conductivity of the sections and the effective thermal conductivity of the structure were determined. This methodology satisfies the test for limit transitions.

1. Introduction

In addition to the long-known allotropic forms of carbon, such as diamond and graphite [1], by the end of the 20th century, carbenes were added (cumulenes - linear structures of the type = C = C = C and polyins –C≡C – C≡C– [2]), linear carbon nanotubes (CNTs) single wall (SWCNTs) and multi wall (MLCNTs) fullerenes — closed single-layer and multi-layer shells, as well as a single-layer carbon sheet structure of graphene [2].

In 2008-2010, joint research of scientists from Tongji and Fudan Universities (China), National Laboratories (Los Alamos National Laboratory, Sandia National Laboratories) and Universities of the US (University of California, Los Angeles; North Carolina State University, Raleigh) discovered a previously unknown form of carbon called "giant" (compared to the size of previously known single wall and multi wall nanotubes) or "colossal" carbon mesotubes (CCT) [3].

The similar previously unknown structures were jointly investigated at the Kutateladze Institute of Thermophysics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia and at the Al-Farabi Institute of Experimental and Theoretical Physics, Kazakhstan [4].
The $D_1$ diameter of the studied SWCNTs is usually in the range of 0.4-40 nm, but the length $L$ can vary in a much wider range - from 1.4 nm to 55.5 cm.

The mechanical and electrical properties of colossal tubes have been investigated at a level sufficient for experimental use, however, the practical absence of data on the thermophysical properties of CCT limits the possibility of their operation in conditions where the thermal regime plays a significant role - in space or on large structures operating in conditions of extreme temperature changes. Due to the lack of data on the thermal conductivity of CCT, the purpose of this work is an analytical assessment of the values of the longitudinal and transverse thermal conductivity of colossal carbon mesotubes.

![Figure 1](image1.png)

**Figure 1.** a) A photograph of colossal carbon tubes (CCT) taken by a scanning electron microscope; b) cylindrical model of the CCT structure with longitudinal channels.

Colossal carbon mesotubes are a two-cylinder coaxial tube-in-tube structure. The outer and inner cylinders (figure 1a) with wall thickness of $\Delta_1$ are interconnected by radial partitions of height $h_p$ and thickness $\Delta_2$, through the $L_3$ gaps (figure 1b). The overall dimensions of CCT depend on the synthesis technology and available equipment. The method of chemical vapor deposition (CVD) produces tubes with a diameter of 40 to 120 $\mu$m and a length of centimeters [3,4].

![Figure 2](image2.png)

**Figure 2.** Model with a square cross-section equal to the cross-sectional area of a cylindrical model: a) with a partition by adiabatic planes a-a parallel to the heat flux and isothermal planes u-u perpendicular to the heat flux.

Carbon tube structures are modeled in the same way as traditional composite structures in which a reinforcing component is surrounded by a matrix component. The concept of a unit cell or Representative Volume Element (RVE) is used to determine the appropriate size and configuration of a computer model to reproduce the mechanical and physical properties of composites. Depending on the subsequent mathematical analysis of the model in polar or Cartesian coordinates, ideal coaxial models with different cross sections of equal area - circular (figure 1b), hexagonal and square (figure 2a) are often used.
Knowing the dimensions of the radial partitions between the outer and inner cylinders and the distance between the interchannel partitions $L_3$, the total number of longitudinal channels $N$ is determined from the condition of equality of the cross-sectional areas of the cylindrical and rectangular models:

$$L_1 = \frac{D_1 \sqrt{\pi}}{2}; \quad N = 4(n-1); \quad n = \frac{L_1 - \Delta}{L_3 + \Delta},$$

where $D_1$ is the outer diameter of the cylindrical mesotube, m; $L_1$ - external size of the model with a square cross-section equal to the cross-sectional area of the cylindrical model, m; $L_3$ - average width of longitudinal channels, m; $\Delta$ - thickness of the wall between longitudinal channels, m; $n$ is the number of longitudinal channels on one side of the square. The model is limited to $n > 3$ by the structure and size of the tube.

An approximate estimate of the values of the effective longitudinal $\lambda_{eff}$ and transverse $\lambda_{eff}$ thermal conductivity will be carried out using the methods of the theory of generalized conductivity using the method of straightening heat flux streamlines proposed by Rayleigh [5].

Let us consider the case when the heat flux is directed along the tube axis. To estimate in the first approximation, let us assume that the transfer along the walls, central and longitudinal channels occurs independently. The formula for the effective longitudinal thermal conductivity is as follows:

$$\lambda_{eff} = \frac{A_{e} \lambda_{IPG} + A_{cc} \lambda_{cc} + A_{lc} \lambda_{lc}}{L_1^2},$$

where $A_{e}$ is the total cross-sectional area of the outer and inner coaxial walls and radial partitions, m$^2$; $A_{cc}$ - cross-sectional area of the central channel, m$^2$; $A_{lc}$ - total cross-sectional area of longitudinal channels, m$^2$; $\lambda_{IPG}$ - longitudinal thermal conductivity of highly oriented pyrographite along the layers (reference data); $\lambda_{cc}$, $\lambda_{lc}$ - are the total, molecular $\lambda_{cmi}$ and radiant $\lambda_{cri}$ components of the thermal conductivity of the gas in the central and longitudinal channels, respectively [5].

$$\lambda_{cc} = \lambda_{cmi} + \lambda_{cri} = \frac{\lambda_{rd}}{1 + \frac{B}{HD_2}} + 2.27 \varepsilon D_1 \left( \frac{T}{100} \right)^3, \quad \lambda_{lc} = \lambda_{cmi} + \lambda_{cri} = \frac{\lambda_{rd}}{1 + \frac{B}{HL_4}} + 2.27 \varepsilon L_3 \left( \frac{T}{100} \right)^3,$$

$$B = \Lambda_\theta H_0 Pr^{(a-1)} \left[ 4\gamma / (\gamma + 1) \right] [(2-a) / a], \quad \gamma = c_p / c_v,$$

where $\Lambda_\theta$ is the average free path of gas molecules at normal pressure $H_0 = 760$ mm Hg; $c_p$, $c_v$ - isobaric and isochoric heat capacity of gas; $Pr$ is the Prandtl number; $a$ is the accommodation coefficient of gas molecules on the surface of a solid.

If there is air in the channels of the mesotubes, then $B = 1.75*10^{-4}[5]$; $H$ - gas pressure in the central and longitudinal channels, mm Hg; $\varepsilon$ - the emissivity of the walls of the central channel and longitudinal channels, for pyrolytic carbon is close to 1.

When analyzing the process of heat transfer in the transverse direction, we use the techniques of the theory of generalized conductivity to straighten heat flux streamlines by systems of auxiliary adiabatic $a-a$ planes and isothermal $u-u$ planes.

Using the system of auxiliary adiabatic $a-a$ planes, we divide the cross-section of the model into separate elementary sections. Using the electrothermal analogy, in which thermal resistances are considered analogs of electrical resistances, individual elementary sections of the model are represented.
in the form of thermal resistances connected to each other in parallel or series circuits, shown in figure 3. The thermal resistance of each of the elementary sections is determined by the expression:

\[ R_i = \frac{L_i}{\lambda_i A_i} \]

If the size of the considered elementary section in the direction of the heat flux is greater than the mean free path of thermal energy carriers, then the thermal conductivity of the substance in this section is assumed to be equal to the reference data. Otherwise, the thermal conductivity of a substance in a given area is determined by the expression:

\[ \lambda(L_i) = \lambda_{rd} \frac{L_i}{\Lambda} \]

where \( \lambda_{rd} \) is the reference value of thermal conductivity, W/(m*K); \( L_i \) - the size of the elementary section in the considered direction, m; \( \Lambda \) is the average mean free path of thermal energy carriers in a given elementary section, m.

The dimensions of the cavity of the central channel and the longitudinal channels between the outer and inner walls determine the intensity of molecular and radiant heat transfer in the transverse direction:

\[ \lambda(r) = \frac{\lambda_{rd}}{1 + \frac{B}{Hr}} + 0.227 \varepsilon r \left( \frac{\bar{T}}{100} \right)^3 \]

where \( r \) is the size of the air cavity in the direction of the heat flux, m; \( \bar{T} \) - average wall temperature, degree of blackness \( \varepsilon \geq 0.9 \).

Let us consider the schemes for connecting the thermal resistances of elementary sections when the model is divided by auxiliary adiabatic planes parallel to the considered direction of the heat flow (figure 3) and isothermal planes perpendicular to the flow (figure 4).

**Figure 3.** Unit cell and resistance circuit in condition the model is divided by adiabatic planes.

**Figure 4.** Unit cell and resistance circuit in condition the model is divided by isothermal planes.

The equivalent thermal resistance is determined for each circuit, when divided by adiabatic planes - \( R_{eqa} \) and isothermal - \( R_{eqi} \). The known value of \( R_{eqa} \) is used to find the effective thermal conductivity of the mesotube in the transverse direction \( \lambda_{ef} \). Then their arithmetic mean value is determined.
Reference data on the properties of highly oriented pyrolytic graphite along $\lambda_{lPG} = 2435$ W/(mK) and across $\lambda_{aPG} = 435$ W/(mK) the layers were used as the initial data on the properties of the wall material. Figure 5 shows the results of predictive estimates.

A model of the structure and a method of analytical (predictive) assessment of the longitudinal and transverse thermal conductivity of colossal carbon tubes of the investigated diameter range $40 < D < 120$ µm are proposed. A fourfold anisotropy of longitudinal and transverse thermal conductivity is revealed.

The high specific strength exceeding the specific strength of carbon nanotubes makes colossal carbon tubes a promising reinforcing component for structures of aviation and space technology, even for a space elevator cable [6], large blades of wind power equipment and for local or personal protective equipment.

![Figure 5. Longitudinal (a) and transversal (b) thermal conductivities.](image)

2. References

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