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Review Article

Cauchy Modeling as a New Trend in Research of Fullerene-Type Nanomaterials

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Abstract

In the work, based on the analysis of heat and gas with acoustic phonons by fullerene, the physical criterion Cauchy is the kind of thermal strength before spring strain, which is caused by the nanotube fullerene

Keywords: Thermal Conductivity; Fullerene; Optimization; Numbers Similarity Numbers

Introduction

Studies of the thermal conductivity of structured nano systems draw attention to the fact that in micro- and nanoelectronics the urgent task of heat dissipation released during the operation of electrical elements [1-6]. So, in the process of electrical switching of the element energy is consumed $\approx 10^{-18} J$, which is on the verge of thermal fluctuations $\approx 0.5 \cdot 10^{-20} J$. This means that a billion (10^9) transistor chip uses order energy in a single act $10^{-3} J$. Then, in order of speed $1 GHz$, the energy consumed can reach values $10^6 \frac{J}{s^{-1}}$, far exceeding the power of a jogging electric kettle $2 \cdot 10^3 \frac{J}{s^{-1}}$.

In order to remove Joule-Lenz heat in electric nanoelements, both microchannels with liquid carriers of heat and conductive elements, such as nanocomposite ceramics filled with carbon nanotubes, can be used, which, depending on their chiral characteristics, can alter the physical properties of nano cells. Thus, it was established [9-12] and confirmed by theoretical estimates [13,14] that the thermal conductivity at room temperature of a carbon nanotube can reach values of $(3 \div 3.5) \cdot 10^3 \frac{J}{s \cdot m \cdot K}$, which significantly exceeds the thermal conductivity of diamon $(1 \div 2.2) \cdot 10^3 \frac{J}{s \cdot m \cdot K}$, which was considered one of the best heat conductors. Carbon nanotubes are thermally stable, characterized by high electrical conductivity [10], high electron mobility [11], and a large specific surface value [15]. It is believed [16] that the abnormally high thermal conductivity of carbon nanotubes is due to their regular structure and the small number of defects and impurity centers in them. In the elementary cell of graphene there are two carbon atoms, so the dispersion spectrum consists of three optical and three acoustic branches, among which the longitudinal and transverse acoustic modes correspond to the speed of sound 2130 and 1360 $\frac{m}{s}$.

If in metals heat is transferred mainly by electrons, then in phononel dielectrics, as quanta of elastic vibrations of a crystal lattice. The speed of the phonons $\frac{d\omega(q)}{d}$ is determined by the slope of the dispersion curve $\omega(q)$, so acoustic phonons are faster than optical ones, and therefore acoustic phonons are the main heat carriers. In [8], the Debye model was supplemented by the idea of quantization of elastic waves, which allowed the problem to be reduced to the problem of phonon gas kinetics modeling. The patterns of phonon thermal energy transport [16] have subsequently led to the creation of nanocomposites, in which, unlike crystalline substances, there is in fact no perfect structure and precise geometry [17]. Therefore, if the composite matrix is filled with graphene, its low-frequency phonons interact with the phonons of the matrix, leading to an increase in the thermal conductivity of the heterogeneous system as a whole [18]. In nanoceramic fillers with fullerene-type structures, the main mechanism of thermal energy transfer is related to acoustic phonons. Acoustic phonons are excited and propagated along carbon nanotubes, so the patterns of heat energy transport will depend on the geometric parameters of carbon nanotubes. Although the main contribution to thermal conductivity is the polymer matrix, it can be adjusted by filling with a metal system with high thermal conductivity, and the use of tubular type carbon nanotubes allows to realize the effect of heat transfer due to the ballistic mechanism of thermal conductivity of phonons, when the losses from acoustic losses. The basic model (Landauer – Datta – Lundstrom transport model or LDL model) of heat energy transfer by phonons, as well as electrons, was developed in work [19]. The authors developed the concept of bottom-up modeling of heat transfer effects in electronic devices as nanoscopic ballistic effect devices. The ballistic mechanism works best in short carbon nanotubes with a length less than the average free path length of the acoustic phonons. Based on the analysis of the results (reference [1-3] in work [20], the author of the work [14] believes that fullerenes, along with high mechanical characteristics, have an increased ability to transfer heat energy to the surface layer itself. The regularity of the transfer of heat energy by solids of small size determines the ratio $\frac{l_m}{L}$, often called the Knudsen number (phonon gas is often compared to classical gas). Here l_m is the length of free path of a phonon in a macroscopic body, whose dimensions are much greater [21]. In nanostructures, parameter L is characteristic dimension, so if $\frac{l_m}{L}\langle 10^{-3}$, then, the diffusion mechanism of heat energy transfer is trueю. If the ratio $\frac{l_m}{L}\rangle\rangle 1 \cong 10^{2}$, known as the so-called Casimir limit, then the magnitude effects become more relevant and the probability of phonon collisions with each other when the phonons propagate from one boundary to the next becomes smaller, that is, in other words, the effect of ballistic heat transfer is enhanced. Therefore, even with an ideal crystalline structure, nanosystems are characterized by a distinct thermal anisotropy of thermal conductivity [22]. In this work, based on a comparative analysis of the thermal conductivity of a carbon nanotube by excitation of acoustic phonons in it, the analysts of the known Cauchy criterion (number) are grounded.

Discussion

In nano systems, transport is determined by the effective electron free path. When the size of the nanoobject becomes smaller than this parameter and becomes commensurate with the de Broglie wave (0.01-0.1 nm), the dependence on the geometric dimensions and shape grows [21]:

$$\lambda_Q(L)=\frac{\lambda_{Q\infty}}{1+\frac{l_\infty}{L}}, \quad (1)$$

where $\lambda_{Q\infty}, l_\infty$ are these are the parameters of a macroscopic body, for example graphite. Then use of similarity criteria makes it possible to carry out preliminary qualitative-theoretical analysis and to make a choice of a system of dimensionless parameters, which are determinable in complex physical processes and allows to properly organize the setting of the experiment and to carry out preliminary processing of results [25]. From the point of view of analysis of models of heat transfer with the participation of acoustic vibrations of atoms and molecules in the medium, the criteria of thermal and mechanical processes attract attention:

Fourier number

$$F_0=\frac{\alpha_T\tau}{L^2}=\frac{\lambda_Q\tau}{\tilde{N}_m\rho_m L^2}, \quad (2)$$

where $\tilde{N}_m\rho_m$ is thermal energy per unit volume of a substance. The physical content of the Fourier criterion is that it determines the ratio of heat flux due to thermal conductivity to local heat flux. In other words, the Fourier criterion is equal to the change in the internal energy in the elementary volume, that is, it describes the relation between the stored energy and that propagated in the medium by the coefficient of thermal conductivity λ_Q. Resizing of L the system causes a slight acceleration of the thermal energy transfer process for a constant Fourier number over a characteristic time τ. Thus, criterion (2) relates the rate of heat propagation to the thermophysical parameters and the size of the carrier (carbon nanotubes in the case of nanoceramics).

Since the inverse value λ_Q^{-1} characterizes thermal inertia, the electromechanical devices of micron-sized thermal effects are also characterized by low thermal inertia. In addition, as follows from (2), the characteristic transition time decreases by the quadratic law from the characteristic geometric parameter (size) of the active element. Therefore, the thermal actuators in the micro- and nanoscale dimensions are characterized by a rather high speed, virtually inertial, such as thermocouples in the form of micro- or nanoscale beams.

Bio number or thermal similarity criterion

$$B=\alpha_T L\lambda_Q^{-1} \quad (3)$$

The number Bio describes the relationship between the temperature gradient between the points at a distance L and the so-called temperature head $\Delta\dot{O}$. In other words, the number Bio describes the ratio of thermal resistance λ_Q^{-1} (similar to the electrical resistance σ_R^{-1} of a section of an electrical circuit with electrical conductivity σ_R and ohmic resistance R) to the thermal resistance of a surface through which heat is dissipated into the environment. The Bio criterion belongs to the group of determining criteria because it includes the coefficient of thermal conductivity of a solid medium. Recall that, in contrast to the Bio criterion, the Nusselt criterion, which includes the coefficient of thermal conductivity of a liquid, refers to the determining criteria.

Cauchy number as a criterion for the ratio of the inertia force to the force of elasticity:

$$Ca = \frac{\rho_m c_S{}^2}{E_\sigma} = \frac{\rho_m \omega^2 L^2}{E_\sigma}, \qquad (3)$$

This criterion characterizes the regularity that the oscillation frequency is inversely proportional to the length, so the natural oscillations of micro- and nano-oscillators are high-frequency, which limits the operating range of electromechanical devices to natural frequencies and causes high dynamic characteristics. Criterion (3) shows that in the case of elastic deformation, the oscillation frequency is inversely proportional to the geometric dimensions of the oscillator. Therefore, micro and nano electromechanical oscillators have a relatively high frequency of resonant oscillations. This allows them not only to significantly improve their dynamic characteristics with a short reaction time, but also to make them insensitive to external acoustic noise. Other similarity criteria are also known [23].

It is known that the thermal conductivity of a status solid is described by the known Fourier equation:

$$\vec{J}_Q = -\lambda_Q \, grad\, T \Rightarrow Q = \lambda_Q S \cdot \frac{\Delta T}{L}\tau . \qquad (4)$$

Руку $\vec{J}_Q$ is the vector of the heat flux density and λ_Q is coefficient of thermal conductivity. By definition, the coefficient of thermal conductivity determines the heat flux $\vec{J}_Q$ in the direction of the space in which there is a temperature gradient, and the minus sign indicates that energy is transferred from the more heated part of the body to the less heated, i.e in the direction of decreasing temperature. Therefore, the temperature gradient $grad\, T$ is a vector quantity directed along the normal to the isothermal surface in the direction of increasing temperature and numerically equal to a partial derivative of the temperature along this direction. Equation (4) is a first order differential equation with respect to t, does not allow for a substitution of time t on the time $-t$, which is proof of the irreversibility of the processes it describes. The right part of it expresses the flux density vector in the form of a scalar gradient. This is a vector, so the flow of a scalar value is also a vector, whereas the flow is already a vector of the tensor. It is the Fourier law that introduces the concept of the coefficient of thermal conductivity. The one-dimensional model of process (4) is shown in Figure 1. As follows from (1) and (2), in the case of nanosystems, these criteria depend on the parameter being affected by the dimensional effect. In the crystal lattice, heat carriers are phonons, as quanta of thermal lattice vibrations. Therefore, in the absence of phonon interaction processes, the heat flux in a crystal is similar to heat transfer by convection in a gas flowing through a cylinder open at the ends. Therefore, the known formula can be applied to the energy of the particle system by concentration n of the phonons:

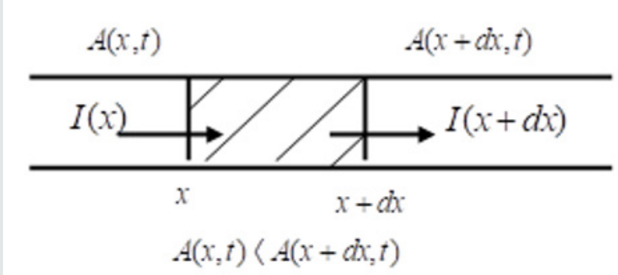

Figure 1: One-dimensional transport model of scalar parameter A(x,t) with intensity I(x,t).

$$W_\vartheta = nk_B T . \qquad (5)$$

In the case of a carbon nanotube, the elastic vibrations of the lattice occur only in the walls of the tube, so the cross-sectional area is the cross-sectional area S of the layer from which the cylinder collapses. It is here that the temperature gradient between the ends of the tube generates phonon gas with energy equivalent to the energy of elastic deformation of the nanowire

$$W_\sigma = S \cdot L \cdot E_\sigma . \qquad (6)$$

For carbon nanotubes with a wall $h \cong d_{C_{60}}$ thickness and radius R, and the Young's Young modulus E_σ of tensile deformation under the action of tensile strength F_L at relative elongation ε is calculated by the formula [26]

$$E_\sigma = \frac{F_L}{2\pi R h \varepsilon} . \qquad (7)$$

According to [27, 28], the characteristic heat transfer time by acoustic phonons in nanostructures is estimated by the formula

$$\tau \cong \frac{m_{C_{60}} \vartheta_S^2}{k_B T} \frac{\omega_{S,\max}}{\omega^2}, \qquad (8)$$

where $\omega_{S,\max}$ is equal to the maximum frequency of acoustic phonons. Then for the relation of energies (4) and (6) taking into account (5) we obtain the formula:

$$\frac{Q}{W_{\sigma\sigma}} = \frac{\lambda_Q \Delta T}{L^2 \cdot E_\sigma}\tau = \frac{\lambda_Q}{k_B}\tau \frac{S}{L} \frac{\frac{\Delta(k_B T)}{L}}{S \cdot E_\sigma} = \qquad (9)$$

$$= \frac{\lambda_Q}{k_B}\tau \frac{F_T}{F_\sigma} \cdot \frac{S}{L} = \frac{\lambda_Q}{k_B}\tau \cdot \mathrm{K}\hat{\iota} \cdot \frac{S}{L}.$$

An analog of the Cauchy criterion $\mathrm{K}\hat{\iota} = \frac{F_T}{F_\sigma}$ is introduced here in the form of the ratio of thermal force $F_T = \frac{\Delta(k_B T)}{L}$ to elastic force $F_\sigma = S \cdot E_\sigma$. In formula (9) records a one-dimensional internal energy gradient propagating in the form of classical elastic waves in a flat layer with a cross-sectional area S and a length L that is folded into a tube. Then, through the elementary volume of the nanotube wall, the length dL and cross-sectional area dS of the nanotube are transmitted over an elementary period of time $d\tau$.

$$dQ = k_B dT = \lambda_Q dS \cdot \frac{dT}{dL} d\tau \Rightarrow \frac{dL}{d\tau} = \vartheta_\sigma =$$
$$= \frac{\lambda_Q}{k_B E_\sigma} d(S \cdot E_\sigma) \Rightarrow F = \frac{\vartheta_\sigma k_B E_\sigma}{\lambda_Q}. \quad (10)$$

The ratio $\frac{1}{\lambda_Q}$ characterizes the so-called thermal resistance, and a similar resistance $\frac{1}{E_\sigma}$ to the propagation of perturbation in the form of elastic deformation. Therefore, it follows from (10) that force resistance to the propagation of local perturbation

$$F = k_B \frac{1/\lambda_Q}{1/E_\sigma} \vartheta_\sigma. \quad (11)$$

is proportional to the velocity that is characteristic of Newton's resistance to physics.

Conclusion

In the work, based on the analysis of heat and gas with acoustic phonons by fullerene, the physical criterion Cauchy is the kind of thermal strength before spring strain, which is caused by the nanotube fullerene.

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