Modeling of second sound in carbon nanostructures

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The study of thermal transport in low-dimensional materials has attracted a lot of attention recently after discovery of high thermal conductivity of graphene. Here we study numerically phonon transport in low-dimensional carbon structures being interested in the hydrodynamic regime revealed through the observation of second sound. We demonstrate that correct numerical modeling of such two-dimensional systems requires semi-classical molecular dynamics simulations of temperature waves that take into account quantum statistics of thermalized phonons. We reveal that second sound can be attributed to the maximum group velocity of bending optical oscillations of carbon structures, and the hydrodynamic effects disappear for \( T > 200 \text{K} \), being replaced by diffusive dynamics of thermal waves. Our numerical results suggest that the velocity of second sound in such low-dimensional structures is about \( 6 \text{ km/s} \), and the hydrodynamic effects are manifested stronger in carbon nanotubes rather than in carbon nanoribbons.

I. INTRODUCTION

Quasi-one-dimensional molecular systems such as carbon nanotubes and two-dimensional atomic layers are known to possess many unusual physical properties. In particular, thermal conductivity in such systems can be unexpectedly high exhibiting unusual phenomena which are important for both fundamental physics and technological applications of graphene and other two-dimensional materials [1–5]. One of such phenomena is associated with second sound, heat waves or hydrodynamic phonon transfer observed at temperatures above 100 K.

In three-dimensional materials, second sound was previously observed experimentally only at cryogenic temperatures [6–10], as a reaction of a material to an applied temperature pulse. Discovered later, exceptionally high thermal conductivities of low-dimensional materials (such as carbon nanotubes and nanoribbons, graphene, and boron nitride) occur due to a ballistic flow of long-wave acoustic phonons supported by such systems [2, 11–15]. Second sound, or hydrodynamic phonon transfer, is observed between ballistic and diffusion regimes of heat transfer. In two-dimensional (2D) materials, second sound can be observed at temperatures above 100K [16–18], and for rapidly changing temperature high-frequency second sound can also be observed in three-dimensional (3D) materials at higher temperatures [19].

To describe the hydrodynamic regime of phonon transfer in low-dimensional materials, several theoretical models were proposed [11, 15, 18, 20–24]. In particular, a 3D model of a periodically modulated graphene structure that behaves like a crystal for temperature waves was proposed in Ref. [25]. Hydrodynamic features of the phonon transfer in a single-wall carbon nanotube with chirality indices (20,20) were discussed in Ref. [26], where the authors suggested a formula for the contribution of phonon drift motion into the total heat flow, and the second sound velocity in the nanotube was estimated as \( v_s = 4\text{ km/s} \). The second sound velocity in the graphene was estimated in Refs. [15, 24] as \( v_s = 3.2\text{ km/s} \) (for temperature 100K).

Direct numerical simulation of second sound in solids is a difficult task because one needs to study polyatomic molecular systems also taking into account quantum statistics of phonons. Propagation of temperature pulses was simulated for single-wall [27–30] and double-wall carbon nanotubes (CNTs) [31] and carbon nanoribbons (CNRs) [32], by employing the classical method of molecular dynamics. This approach predicts thermalization of all phonons regardless of their frequency and temperature. The thermal pulse was generated by connecting a short edge section of a nanotube (or a nanoribbon) with a thermostat at temperature \( T_h = 800\text{K}, \) or 1000K for a short time (\( \sim 1\text{ ps} \)). Either a zero value [27, 29–31] or \( T = 50 K \) [28, 32] was used as a background temperature. The motion of a thermal pulse along the nanotube was analyzed through the study of spatiotemporal temperature profiles. It was shown that the initial thermal pulse

\[ \text{FIG. 1: Motion of a heat pulse along a carbon nanotube with chirality index (6,6). Case (a) is the initial condition at } t = 0. \text{ Cases (b,c) show schematically the temperature distribution along the nanotube for two different scenarios of heat transfer: (b) spreading, for high temperature } T = 300K, \text{ (c) propagation of a heat wave, for low temperature } T = 50, \text{ where } v_s \text{ is the speed of second sound.} \]
causes the formation of several wave packets, the leading one moving at the speed of long-wave acoustic phonons.

In this paper, we study the propagation of thermal pulses along carbon nanotubes and carbon nanoribbons (see Fig. 1) by using semi-classical molecular dynamic simulations [33]. This approach allows us to model thermalized phonons also taking into account their quantum statistics, i.e., taking into account the full thermalization of low-frequency phonons with frequencies $\omega < k_B T/\hbar$ and partial thermalization of phonons with frequencies $\omega > k_B T/\hbar$, where $k_B$ is the Boltzmann constant, $\hbar$ is the Planck constant. As we demonstrate below, our approach allows to simulate second sound in graphene at $T \approx 100\text{K}$ only taking into account quantum statistics of phonons. In that way, we can study not only the propagation of a short thermal pulse but also the dynamics of periodic sinusoidal temperature profiles, as relaxation of the periodic temperature lattices.

The paper is organized as follows. Section II describes our full-atomic model of carbon nanoribbons and carbon nanotubes, which is further employed to simulate numerically the heat transport. In Sec. III, we construct the dispersion curves of nanoribbons and nanotubes, and analyze their characteristics and the propagation velocities of low-frequency phonons. Section IV describes our method of semi-classical molecular dynamics simulations. Then in Sec. V, we simulate numerically different regime of the propagation of a thermal pulse, and in Sec. VI we study relaxation of temperature periodic lattices. More specifically, we demonstrate the existence of second sound for temperatures $50 \div 150\text{K}$. In Sec. VII, for a direct comparison, we study the dynamics of thermal pulses and relaxation of periodic temperature lattices by employing the classical molecular dynamics. Section VIII concludes our paper. Thus, we reveal that the quantum statistics of phonons should be taken into account for the study of second sound in low-dimensional systems.

II. MODEL

We consider a planar carbon nanoribbon (CNR) and a nanotube (CNT) with a zigzag structure consisting of $N \times K$ atoms – see Fig. 2 ($N$ is the number of transverse unit cells, $K$ – the number of atoms in the unit cell). The nanoribbon is assumed to be flat in the ground state. Initially, we assume that the nanoribbon lies in the $xy$ plane, and its symmetry center is directed along the $x$ axis. Then its length can be calculated as $L_x = (N - 0.5)a$, width $L_y = 3Kr_0/4 - r_0$, where the longitudinal step of the nanoribbon is $a = r_0 \sqrt{3}$, $r_0 = 1.418 \text{Å}$ – C–C valence bond length.

In realistic cases, the edges of the nanoribbon are always chemically modified. For simplicity, we assume that the hydrogen atoms are attached to each edge carbon atom forming the edge line of CH groups. In our numerical simulations, we take this into account by a change of the mass of the edge atoms. We assume that the edge carbon atoms have the mass $M_1 = 13m_p$, while all other internal carbon atoms have the mass $M_0 = 12m_p$, where $m_p = 1.6601 \times 10^{-27} \text{kg}$ is the proton mass.

Hamiltonian of the nanoribbon and nanotube can be presented in the form,

$$
H = \sum_{n=1}^{N} \sum_{k=1}^{K} \left[ \frac{1}{2} M_{n,k} \dot{\mathbf{u}}_{n,k} \cdot \dot{\mathbf{u}}_{n,k} + P_{n,k} \right],
$$

where each carbon atom has a two-component index $\alpha = (n,k)$, $n$ is the number of transversal elementary cell of zigzag nanoribbon (nanotube), $k$ is the number of atoms in the cell. Here $M_{n,k}$ is the mass of the carbon atom with the index $\alpha$ (for internal atoms of nanoribbon and for all atoms of nanotube, $M_{n,k} = M_0$, for the edge atoms of nanoribbon, $M_{n,k} = M_1$), $\mathbf{u}_\alpha = (x_\alpha(t), y_\alpha(t), z_\alpha(t))$ is the three-dimensional vector that describes the position of an atom with the index $\alpha$ at the time moment $t$. The term $P_{n,k}$ describes the interaction of the carbon atom with the index $\alpha$ with the neighboring atoms. The po-

FIG. 2: Atomic model of (a) carbon zigzag nanoribbon and (b) nanotube with chirality index (6,6). Nanoribbon and nanotube are placed along the $x$ axis, $a$ is longitudinal step, $n$ is number of transverse unit cells (dashed lines separate unit cells), and the number atoms in the unit cell $K = 24$. 
tential depends on variations in bond length, in bond
angles, and in dihedral angles between the planes formed
by three neighboring carbon atoms. It can be written in
the form

\[ P = \sum_{\Omega_1} U_1 + \sum_{\Omega_2} U_2 + \sum_{\Omega_3} U_3 + \sum_{\Omega_4} U_4 + \sum_{\Omega_5} U_5, \]

where \( \Omega_i \), with \( i = 1, 2, 3, 4, 5 \), are the sets of configu-
ration including all interactions of neighbors. These sets
only need to contain configurations of the atoms shown in
Fig. 3, including their rotated and mirrored versions.

Potential \( U_1(u_{\alpha}, u_{\beta}) \) describes the defor-
mation energy due to a direct interaction between pairs of atoms
with the indexes \( \alpha \) and \( \beta \), as shown in Fig. 3(a). The potential \( U_2(u_{\alpha}, u_{\beta}, u_{\gamma}) \) describes the defor-
mation energy of the angle between the valence bonds
\( u_{\alpha}u_{\beta} \), and \( u_{\beta}u_{\gamma} \), see Fig. 3(b). Potentials \( U_i(u_{\alpha}, u_{\beta}, u_{\gamma}) \), \( i = 3, 4 \), and 5,
describe the deformation energy associated with a change
in the angle between the planes \( u_{\alpha}u_{\beta}u_{\gamma} \) and \( u_{\beta}u_{\gamma}u_{\delta} \), as shown in Figs. 3(e)–(e).

We use the potentials employed in the modeling of the
dynamics of large polymer macromolecules \([34, 35]\)
for the valence bond coupling,

\[ U_1(u_1, u_2) = \epsilon_1 \{ \exp[-\alpha_0 (\rho - \rho_0)] - 1 \}^2, \rho = |u_2 - u_1|, \]

where \( \epsilon_1 = 4.9632 \) eV is the energy of the valence bond
and \( \rho_0 = 1.1418 \) Å is the equilibrium length of the bond;
the potential of the valence angle

\[ U_2(u_1, u_2, u_3) = \epsilon_2 (\cos \phi - \cos \phi_0)^2, \]

\[ \cos \phi = \frac{\langle u_3 - u_2, u_1 - u_2 \rangle }{\| u_3 - u_2 \| \cdot \| u_2 - u_1 \|}, \]

so that the equilibrium value of the angle is defined as
\( \cos \phi_0 = \cos(2\pi/3) = -1/2 \); the potential of the torsion angle

\[ U_i(u_1, u_2, u_3, u_4) = \epsilon_i (1 + z_i \cos \psi), \]

\[ \cos \psi = \frac{\langle v_1, v_2 \rangle }{\| v_1 \| \cdot \| v_2 \|}, \]

\[ v_1 = (u_2 - u_1) \times (u_3 - u_2), \]

\[ v_2 = (u_3 - u_2) \times (u_4 - u_3), \]

where the sign \( z_i = 1 \) for the indices \( i = 3, 4 \) (equilibrium
value of the torsional angle \( \phi_0 = \pi \)) and \( z_i = -1 \) for the
index \( i = 5 \) (\( \phi_0 = 0 \)).

The specific values of the parameters are \( \alpha_0 =
1.7889 \) Å\(^{-1} \), \( \epsilon_2 = 1.3143 \) eV, and \( \epsilon_3 = 0.499 \) eV, they are
found from the frequency spectrum of small-amplitude
oscillations of a sheet of graphite \([36]\). According to pre-
vious study \([37]\), the energy \( \epsilon_4 \) is close to the energy \( \epsilon_3 \),
whereas \( \epsilon_5 \ll \epsilon_4 \) (\( |\epsilon_5/\epsilon_4| < 1/20 \)). Therefore, in what
follows we use the values \( \epsilon_4 = \epsilon_3 = 0.499 \) eV and assume
\( \epsilon_5 = 0 \), the latter means that we omit the last term in
the sum (2). More detailed discussion and motivation of
our choice of the interaction potentials (3), (4), (5) can
be found in earlier publication \([38]\).

III. DISPERSION CURVES

Let us consider carbon nanoribbon (nanotube) in the
equilibrium state \( \{u_{n,k}^0\}_{n,K=-\infty}^{+\infty} \) which is characterised
by longitudinal shift \( a \) and by the positions of \( K \) atoms
in the elementary cell: \( u_{n,k}^0 = u_{0,k}^0 + an \mathbf{e}_x \), where vector
\( e_x = (1, 0, 0) \) — see Fig. 2.

Then, we introduce 3K-dimensional vector,
\( \mathbf{v}_n = (u_{n,k}^0 - u_{0,k}^0)^K_{k=1} \), that describes a shift of the atoms of the
nth cell from its equilibrium positions. The nanoribbon
(nanotube) Hamiltonian can be written in the following form:

\[ H = \sum_n \left\{ \frac{1}{2} (\mathbf{M} \ddot{\mathbf{v}}_n, \dot{\mathbf{v}}_n) + P(v_{n-1}, v_n, v_{n+1}) \right\}, \]

where \( \mathbf{M} \) is the diagonal matrix of masses of all atoms of the
elementary cell.

Hamiltonian (6) generates the following set of the equa-
tion of motion:

\[ -\mathbf{M} \ddot{\mathbf{v}}_n = P_1(v_n, v_{n+1}, v_{n+2}) + P_2(v_{n-1}, v_n, v_{n+1}) + P_3(v_{n-2}, v_{n-1}, v_n), \]

where function

\[ P_i(v_1, v_2, v_3) = \frac{\partial}{\partial v_i} P(v_1, v_2, v_3), \quad i = 1, 2, 3. \]

In the linear approximation, this system takes the form

\[ -\mathbf{M} \ddot{\mathbf{v}}_n = \mathbf{B}_1 \mathbf{v}_n + \mathbf{B}_2 \mathbf{v}_{n+1} + \mathbf{B}_2^\prime \mathbf{v}_{n-1} + \mathbf{B}_3 \mathbf{v}_{n+2} + \mathbf{B}_3^\prime \mathbf{v}_{n-2}, \]

where the matrix elements are defined as

\[ \mathbf{B}_1 = \mathbf{P}_{1,1} + \mathbf{P}_{2,2} + \mathbf{P}_{3,3}, \quad \mathbf{B}_2 = \mathbf{P}_{1,2} + \mathbf{P}_{2,3}, \quad \mathbf{B}_3 = \mathbf{P}_{1,3}, \]

and the matrix of the partial derivatives takes the form

\[ \mathbf{P}_{i,j} = \frac{\partial^2 P}{\partial v_i \partial v_j}(0, 0, 0), \quad i, j = 1, 2, 3. \]

Solution of the system linear equations (8) can be written
in the standard form of the wave

\[ \mathbf{v}_n = \mathbf{A} \exp(\mathbf{i}q n - \mathbf{i} \omega t), \]

where \( \mathbf{A} \) — amplitude, \( \mathbf{w} \) — eigenvector, \( \omega \) is phonon fre-
quency with the dimensionless wave number \( q \in [0, \pi] \).
Substituting Eq. (9) into Eq. (8), we obtain the eigen-
value problem

\[ \omega^2 \mathbf{M} \mathbf{w} = \mathbf{C}(q) \mathbf{w}, \]

Fig. 3: Configurations containing up to ith type of nearest-
neighbor interaction for (a) \( i = 1 \), (b) \( i = 2 \), (c) \( i = 3 \), (d)
\( i = 4 \), and (e) \( i = 5 \).
where Hermitian matrix
\[
C(q) = B_1 + B_2e^{iq} + B_2^*e^{-iq} + B_3e^{2iq} + B_3^*e^{-2iq}.
\]
Using the substitution \(\mathbf{w} = \mathbf{M}^{-1/2}\mathbf{e}\), problem (10) can be rewritten in the form
\[
\omega^2\mathbf{e} = \mathbf{M}^{-1/2}C(q)\mathbf{M}^{-1/2}\mathbf{e}, \tag{11}
\]
where \(\mathbf{e}\) is the normalized eigenvector, \((\mathbf{e}, \mathbf{e}) = 1\).

Therefore, in order to find the dispersion relations characterizing the modes of the nanoribbon (nanotube) for each fixed value of the dimensionless wave number \(0 \leq q \leq \pi\) we need to find numerically the eigenvalues of the Hermitian matrix [Eq. (11)] of the order \(3K \times 3K\). As a result, we obtain \(3K\) branches of the dispersion curve \((\omega_j(q))_{j=1}^{3K}\).

The plain structure of the nanoribbon allows us to divide its vibrations into two classes: into in-plane vibrations, when the atoms always stay in the plane of the nanoribbon and into out-of-plane vibrations when the atoms are shifted orthogonal to the plane. Two third of the branches correspond to the atom vibrations in the \(xy\) plane of the nanoribbon (in-plane vibrations), whereas only one third corresponds to the vibrations orthogonal to the plane (out-of-plane vibrations), when the atoms are shifted along the axes \(z\). The maximal frequency of in-plane vibrations is \(\omega_m = 1598\ \text{cm}^{-1}\), the maximum frequency of out-of-plane vibrations is \(\omega = 898\ \text{cm}^{-1}\).

This values goes in accord with the experimental data for planar graphite [39–41].

The form of nanoribbon dispersions curves in the low frequency region is shown in Fig. 4. Four branches of the curves start from the zero point \((q = 0, \omega = 0)\). Two first branches \(\omega_1(q), i = 1, 2\) correspond to the orthogonal (out-of-plane) bending vibrations of the nanoribbon; third branch \(\omega_3(q)\) describes the bending planar (in-plane) vibrations in the plane. These branches approach smoothly the axis \(q: \omega_i(q)/q \to 0\), when \(q \to 0\), so that the corresponding long-wave phonon possess zero dispersion. However, we can determine for them the maximum values of group velocities
\[
s_i = a \max_{0 \leq q \leq \pi} d\omega_i(q)/dq, \quad i = 1, 2, 3.
\]
Forth branch \(\omega_4(q)\) correspond to in-plane longitudinal vibrations. The corresponding long-wave mode posses nonzero dispersion so that we can define limiting value
\[
v_l = a \lim_{q \to 0} \omega_4(q)/q = 13.36\ \text{km/s},
\]
which define the sound speed of longitudinal acoustic waves (phonons) of the nanoribbon. The speeds of optical (bending) phonons will determine the values \(v_o = s_1, s_2 = 5.88\ \text{km/s}\) for out-of-plane and \(v_t = s_3 = 7.79\ \text{km/s}\) for in-plane vibrations – see Fig. 4 (b).

The maximal frequency of nanotube vibrations \(\omega_m = 1630\ \text{cm}^{-1}\). The form of dispersion curve in the low frequency region is shown in Fig. 5. For nanotube four branches of the curve also start from zero point. Two
first branches $\omega_i(q)$, $i = 1, 2$ correspond to the bending vibrations. These branches approach smoothly the axis $q$: $\omega_i(q)/q \to 0$, when $q \to 0$ (corresponding long-wave binding phonon posses zero dispersion). For them we can determine the maximum values of group velocities

$$v_g = a \max_{q \in [0, \pi]} \omega_i(q)/dq = 6.54 \text{ km/s}.$$ 

Third and forth branches correspond to torsional and longitudinal acoustic phonon of the nanotube. The corresponding long-wave modes posses nonzero dispersion so that we can define limiting values

$$s_i = a \lim_{q \to 0} \omega_i(q)/q, \quad i = 3, 4,$$

which define the sound speed of acoustic torsional $v_t = s_3 = 8.41 \text{ km/s}$ and longitudinal waves $v_l = s_4 = 13.84 \text{ km/s}$ – see Fig. 5(b).

Let us note that when taking into account the quantum statistics of thermal phonons, only nonzero phonons with the average energy of $k_B T p(\omega, T)$ can participate in heat transfer, where the degree of thermalization

$$p(\omega, T) = \frac{\hbar \omega/k_BT}{\exp(\hbar \omega/k_BT) - 1},$$

depends on temperature $T$ and phonon frequency $\omega$ (function $0 < p(\omega, T) < 1$). $k_B$ and $\hbar$ are the Boltzmann and Planck constants [42]. Here it is taken into account that zero-point oscillations are not involved in the heat phonon transport.

As the temperature increases, $T \to \infty$, density $p \to 1$. At high temperatures, all phonons become equally thermalized, each has the average energy equal to $k_B T$ (classical approximation). When the temperature decreases, high-frequency nonzero phonons freeze out ($p(\omega, T) < 0$ when $T \to 0$), only phonons with frequencies $\omega < \Omega(T)$ where thermalization frequency

$$\Omega(T) = k_B T/\hbar,$$

remain thermalized [function $p(\Omega(T), T) = 1/(e - 1) = 0.582$]. Therefore, at low temperatures, only low-frequency phonons will participate in heat transfer.

Thus, at $T < 400\text{K}$, phonons with frequencies $\omega < 300 \text{ cm}^{-1}$ will participate in heat transfer, and at $T < 50\text{K}$ it will be only low-frequency long-wave phonons (see Figs. 4 and 5). The degree of participation of a phonon with a frequency of $\omega$ in heat transfer is characterized by the function (12).

\section{IV. INTERACTION WITH A THERMOSTAT}

In the classical approach interaction of nanoribbons (nanotubes) with a thermostat is described by the Langevin system of equations

$$M\ddot{\mathbf{x}}_n = -\frac{\partial H}{\partial \mathbf{x}_n} - \gamma M\dot{\mathbf{x}}_n + \Xi_n, \quad 1 \leq n \leq N,$$

where $M$ is $3K \times 3K$-dimensional diagonal mass matrix, $3K$-dimensional vector $\mathbf{x}_n = \{u_{n,k}\}_{k=1}^3$ gives the coordinates of carbon atoms from $n$th transverse unit cell, damping coefficient $\gamma = 1/t_0$ ($t_0$ – relaxation time) and $\Xi_n = \{\xi_{n,k}\}_{k=1}^3$ is $3K$-dimensional vector of normally distributed random forces (white noise) normalized by conditions

$$\langle \xi_{\alpha,i}(t_1)\xi_{\beta,j}(t_2) \rangle = 2M_\alpha \gamma k_B T \delta_{\alpha\beta}\delta_{ij}\delta(t_1 - t_2).$$

In the semiquantum approach the random forces do not represent in general white noise. The power spectral density of the random forces in that description should be given by the quantum fluctuation-dissipation theorem [42, 43]:

$$\langle \xi_{\alpha,i}(t_1)\xi_{\beta,j}(t_2) \rangle = 2M_\alpha \gamma k_B T \delta_{\alpha\beta}\delta_{ij}p(\omega, T).$$

To model the nanoribbon (nanotube) stochastic dynamics in the semiquantum approach [33], we will use the Langevin equations of motions (13) with random forces $\Xi_n = \{\xi_{n,k}\}_{k=1}^3$ with the power spectral density, given by $p(\omega, T)$, where $T_n$ is temperature of the $n$th transverse unit cell. This dimension color noise $\xi_n$ is conveniently derived from the dimensionless noise $S_{n\alpha}(\tau)$: $\xi_n(t) = k_BT_n\sqrt{2M_\alpha \gamma /\hbar}S_{n\alpha}(\tau)$, where dimensionless time $\tau = k_BT_n t/\hbar$, spectral density

$$p_1(\omega) = \omega/(\exp(\omega) - 1),$$

dimensionless frequency $\bar{\omega} = \hbar \omega/k_BT_n$.

The random function $S_{n\alpha}(\tau)$, which will generate the power spectral density $p_1(\bar{\omega})$, can be approximated by a sum of two random functions with narrow frequency spectra:

$$S_{n\alpha}(\tau) = c_1S_{1,n\alpha}(\tau) + c_2S_{2,n\alpha}(\tau).$$

In this sum the dimensionless random functions $S_{i,n\alpha}(\tau), \quad i = 1, 2$, satisfy the equations of motion as

$$\ddot{\xi}_{n\alpha}(\tau) = \eta_{n\alpha}(\tau) - \bar{\Gamma}_{n\alpha}(\tau) - \bar{\Gamma}^{\prime}\xi_{n\alpha}(\tau),$$

where $\eta_{n\alpha}(\tau)$ are $\delta$-correlated white-noise functions:

$$\langle \eta_{n\alpha}(\tau)\eta_{j,k\beta}(0) \rangle = 2\bar{\Gamma}_{i,j}\delta_{nk}\delta_{\alpha\beta}\delta(\tau).$$

The power spectral density of the sum of two random functions (17) $S_{n\alpha}S_{k\beta}$ is $\delta_{nk}\delta_{\alpha\beta}p_2(\bar{\omega})$, where function

$$p_2(\bar{\omega}) = \frac{2c_1^2c_2^2}{(\Omega_n^2 - \bar{\omega}^2)^2 + \bar{\omega}^2\Gamma_n^2}.$$

The function $p_2(\bar{\omega})$ approximate with high accuracy the function $p_1(\bar{\omega})$ for the values of dimensionless parameters $c_i, \Omega_i, \Gamma_i, \quad i = 1, 2$ represented in Table 1.

Thus, in order to obtain the thermalized state of the nanoribbon (nanotube), it is necessary to solve numerically the system of equation of motion with color noise:

$$M\ddot{x}_n = -\frac{\partial H}{\partial x_n} - \gamma M\dot{x}_n + c_1\Theta_{1,n} + c_1\Theta_{2,n}, \quad 1 \leq n \leq N,$$
where $3K$-dimensional vector of random forces $\Theta_{i,n} = \{\zeta_{i,n,k,j}\}_{k,j=1}^{3K}$, $i = 1, 2$, is a solution of system of linear equations

$$\ddot{\zeta}_{i,n,\alpha} = \eta_{i,n,\alpha} - \left(\frac{\Omega_i}{\hbar} - \Delta \Gamma_i\right) \zeta_{i,n,\alpha} - \frac{\hbar}{\Omega_i} \dot{\zeta}_{i,n,\alpha}, \quad i = 1, 2,$$

(21)

where $\eta_{i,n,\alpha}$ are normally distributed random forces (white noise) normalized by conditions

$$\langle \eta_{i,n,\alpha}(t)\eta_{j,k,\beta}(0) \rangle = 4\tilde{\Gamma}_i \left(\frac{\hbar B T_n}{\hbar}\right)^5 \hbar \gamma M_n \delta_{ij} \delta_{nk} \delta(t). \quad (22)$$

The system of equations (20), (21) was integrated numerically with the initial conditions

$$x_n(0) = x_n^0, \quad \dot{x}_n(0) = 0, \quad \Theta_{i,n} = 0, \quad \dot{\Theta}_{i,n} = 0 \quad (23)$$

$n = 1, 2, ..., N, \quad i = 1, 2,$

where $x_n^0$ is the coordinate of carbon atoms in ground stationary state of nanoribbon (nanotube). The value of the relaxation time $t_0$ characterizes the intensity of the exchange of the molecular system with the thermostat. To achieve the equilibrium of the system with the thermostat, it is enough to integrated the system of equations of motion during the time $t = 10t_0$.

In the simulation, the value $t_0 = 0.4$ ps was used. The system equations (20), (21) was integrated numerically during the time $t_1 = 5$ ps. Further the interaction with the thermostat was turned off, i.e. the system of equations of motion without friction and random forces

$$\mathbf{M}\ddot{x}_n = -\frac{\partial H}{\partial x_n}, \quad n = 1, 2, ..., N, \quad (24)$$

was numerically integrated.

Without taking into account zero-point oscillations, the normalized kinetic energy of thermal phonons

$$e(T) = \frac{1}{3NK} \sum_{n=1}^{3NK} \hbar \Omega_n \exp(\hbar \Omega_n / \hbar B T) - 1, \quad (25)$$

where $\{\Omega_n\}_{n=1}^{3NK}$ are the nonzero natural oscillations frequencies of the nanoribbon (nanotube). The average value of kinetic energy can also be obtained from the integration of a thermalized system of equations of motion (24)

$$e_{kin} = \frac{1}{3NK} \langle \mathbf{M}\dot{x}_n(0), \mathbf{M}\dot{x}_n(0) \rangle = \frac{1}{3NK} \int_0^t \sum_{n=1}^{N} \langle \mathbf{M}\dot{x}_n(s), \mathbf{M}\dot{x}_n(s) \rangle ds. \quad (26)$$

For a uniformly thermalized molecular system, these energies must coincide:

$$e(T) = e_{kin}. \quad (27)$$

Since function $e(T)$ monotonically increases with $T$, Eq. (27) has a unique solution for the temperature. For inhomogeneous thermalization, the solution of the equation

$$e(T_n) = \frac{1}{3K} \langle \mathbf{M}\dot{x}_n(0), \mathbf{M}\dot{x}_n(0) \rangle \quad (28)$$

allows us to find the distribution of temperature along the nanoribbon (nanotube) $\{T_n\}_{n=1}^N$.

In classical approach, i.e. by using a system of Langevin equations (13) with white noise (14), the temperature distribution can be obtained from the formula

$$T_n = \frac{1}{3K} \langle \mathbf{M}\dot{x}_n(0), \mathbf{M}\dot{x}_n(0) \rangle \quad (29)$$

V. DYNAMICS OF A THERMAL PULSE

Let us simulate the propagations of a thermal impulse along carbon nanoribbon (CNR) and nanotube (CNT) at different values of background temperature. For this purpose, we take the finite CNR and CNT presented in Fig. 2 consisting of $N = 10000$ transversal cells with fixed ends: $x_1 = 0, x_N = 0$.

Then we take CNR (CNT) in the ground stationary state and thermalize it so that the first $N_1 = 40$ unit cells have a higher temperature than remaining cells. For this purpose, we integrate Langevin’s system of equations of motion with color noise (20), (21) with the initial temperature distribution:

$$\{T_n = T_h\}_{n=1}^{N_1}, \quad \{T_n = T\}_{n=N_1+1}^N \quad (30)$$

where the temperature of the left edge is higher than the temperature of the main part of CNR (CNT) ($T_h > T$).

After integrating the system of equations of motion (20), (21) during the time $t_1 = 5$ ns, we will have the thermalized state of the system

$$\{x_n(t_1), \mathbf{M}\dot{x}_n(t_1)\}_{n=1}^N \quad (31)$$

in which all phonons of the nanoribbon (nanotube) will be thermalized according to their quantum statistics (12) (with almost complete thermalization of low-frequency and partial thermalization of high-frequency phonons). Next, we disable the interaction of the molecular system with the thermostat, i.e. we already integrate the system of Hamilton equations (24) with the initial condition (31). Using the formula (28), we will monitor the change of temperature profile along CNR (CNT) $\{T_n(t)\}_{n=1}^N$. To increase the accuracy, the temperature profile is determined by $10^3$ independent realisations of the initial thermalized state of the molecular system.
FIG. 6: Dynamics of the temperature impulse along nanoribbon (width $L_y = 2.41$ nm) at its initial temperature $T_h = 3T$, length $N_t = 40$ and background temperature (a) $T = 50$, (b) 100 and (c) 300 K. The dependence of the temperature distribution along the CNR $T_n$ on the time $t$ is shown. The dashed (red) lines shows trajectories for moving with constant speed $v = v_o, v_t$ and $v_l$.

Modeling the propagation of an initial narrow temperature pulse ($N_t = 40, T_h = 3T$) along the nanoribbon has shown that at low temperatures $50 \leq T \leq 100$K, the thermal vibrations propagate along the nanoribbon as a clearly visible wide wave the maximum of which moves at a speed of $v = v_o$ – see Fig. 6 (a,b). The value of the wave motion velocity suggests that the main role in its formation is played by bending thermal phonons. Therefore, here the velocity of the second sound corresponds to the maximum group velocity of the optical bending phonons of the nanoribbon. At a higher temperature $T > 100$K, no temperature waves are formed, we see only a slow expansion of the initial temperature impulse – see Fig. 6 (c). Such dynamics is typical for the diffusion regime of heat transfer.

In the nanotube, the motion of heat waves is more pronounced – see Fig. 7 (a,b). For $50 \leq T \leq 150$K, two waves are clearly distinguished: a stable localized wave moving at the speed of acoustic long-wave torsional phonons $v_t$ and a wider wave moving at the maximum speed of optical bending phonons $v_o$. The first wave corresponds to the ballistic regime of heat transfer, and the second wave – to the second sound (to hydrodynamic regime of heat transfer). As the temperature increases, the heat waves become subtle. At $T = 300$K, the first (ballistic) wave becomes barely noticeable, and the second quickly disappears. Here, the temperature propagates along the nanotube in the form of a diffusive expansion of the initial impulse – see Fig. 7 (c). Let us note that an increase in the amplitude of the initial temperature impulse $T_h$ does not lead to an increase in the proportion of energy carried by heat waves. On the contrary, an increase in $T_h$ leads to the propagation of energy in the form of a diffusive expansion of the initial temperature pulse even at a small value of the background
FIG. 8: Dynamics of the temperature impulse along CNT (6,6) at its initial temperature (a) \( T_h = 200 \), (b) 500 and (c) 900 K (\( T = 100 \text{K}, N_t = 40 \)). The dependence of the temperature distribution along the CNT \( T_n \) on the time \( t \) is shown. The dashed (red) lines show trajectories for moving with constant speed \( v = v_0, v_t \) and \( v_l \).

temperature \( T \) – see Fig. 8 and Fig. 7 (b).

VI. RELAXATION OF A PERIODIC THERMAL LATTICE

The second sound can also be determined from the relaxation scenario of the initial periodic sinusoidal temperature profile (from the relaxation of the temperature lattice). Note that in the experimental works [16, 17] the second sound in graphite was determined from the analysis of relaxation of the temperature lattice.

Consider the finite nanoribbon (nanotube) of the length 2012 nm (number of unit cells \( N = 2^{13} = 8192 \)) with periodic boundary conditions. In order to study the relaxation of the initial periodic temperature distribution let us consider dynamic of CNR (CNT) with sinusoidal temperature profile

\[
\{T_n = T + \Delta T \cos[2\pi(n - 1)/Z]\}_{n=1}^N,
\]

(32)

where \( T \) is the average temperature, \( \Delta T \) is the profile amplitude, and \( Z = 2^{4+l}, l = 0, \ldots, 7 \) is dimensionless period of the profile.

To obtain the initial thermalized state, we numerically integrate the Langevin system of equations with color noise \((20), (21)\) with temperature distribution \((32)\) during the time \( t_1 = 5 \text{ ps} \). Then we use the resulting normalized state CNR (CNT) \((31)\) as the starting point for the Hamiltonian system equations of motion \((24)\). As a result of numerical integration of this system, using the formula \((28)\), we have the time dependence of the temperature distribution along the nanoribbon (nanotube) \( \{T_n(t)\}_{n=1}^N \). To increase accuracy, the results were averaged over \( 10^4 \) independent realizations of the initial
FIG. 10: Evolution of the relaxation temperature profile in the zigzag nanoribbon with width \( L_y = 2.41 \) nm (length \( N = 2^{13} \)) for period \( Z = 2^{4+i} \) \( (i = 0, 1, ..., 7) \) for (a) temperature \( T = 100\text{K} \) (\( \Delta T = 50\text{K} \)) and (b) \( T = 300\text{K} \) (\( \Delta T = 150\text{K} \)). Time dependencies of the mode maximum \( T(1) \) [blue lines] and of minimum \( T(1 + Z/2) \) [red lines] are depicted. Time scales are differ for each curve in order to fit them into one figure, time \( t_0 = 0.04 \) ps.

FIG. 11: Relaxation of initial periodic thermal profile (temperature lattice) in the CNT (6,6) for temperature (a) \( T = 100\text{K} \) (\( \Delta T = 50\text{K} \)) and (b) \( T = 300\text{K} \) (\( \Delta T = 150\text{K} \)). The period of the profile \( Z = 2^{11} \), nanoribbon length \( N = 2^{13} \). The temperature change on three periods of the profile is shown. The initial temperature distribution in CNT is shown at the top of each figure.

thermalized state of the molecular system.

Let us take two values of the average temperature \( T = 100, \) 300K and the lattice amplitude \( \Delta T = 0.5T \). The results of numerical simulation of the relaxation of the temperature lattice in the nanoribbon are shown in Fig. 9 and 10, and in the nanotube – in Fig. 11 and 12.

As can be seen from Fig. 9, at the profile period \( Z = 2^{11} \), damped periodic fluctuations of the temperature profile occur in the nanoribbon at low temperature \( T = 100\text{K} \). Such behavior corresponds to the hydrodynamic regime of heat transfer. The speed of the temperature wave can be determined from the oscillation period \( t_p \): \( v(Z) = aZ/t_p \). Damped profile fluctuations occur for all its considered periods \( Z = 2^{4}, 2^{5}, ..., 2^{11} \) – see Fig. 10. At \( T = 300\text{K} \) there are no periodic fluctuations. We only see a smooth spreading of the initial temperature profile. This behavior is typical for the diffusion regime of heat transfer.

The typical behavior of the temperature profile in a nanotube is shown in Fig. 11. As can be seen from the figure, when the profile period is \( Z = 2^{11} \) and the temperature is \( T = 100\text{K} \), slowly attenuating periodic profile oscillations occur in the nanotube. This behavior corresponds to the hydrodynamic regime of heat transfer. Profile fluctuations occur at all considered values of its period \( Z = 2^{4}, 2^{5}, ..., 2^{11} \) – see Fig. 12. At \( T = 300\text{K} \) low-amplitude profile fluctuations are noticeable only for \( Z \leq 2^{9} \). Here, an increase in the profile period leads to a rapid transition of the profile dynamics to the diffusion regime. We can say that at \( T = 300\text{K} \), the second sound can manifest itself only at the lengths \( L \leq 2^{9}a = 125.7 \) nm.

The dispersion of temperature waves at a temperature of \( T = 100\text{K} \) is shown in Fig. 13. With the increase of wavelength \( L = aZ \), its velocity \( v(Z) \) monotonically decreases and in the limit tends to the maximum group velocity of optical bending phonons \( v_0 \). Therefore, in car-
bon nanoribbons and nanotubes, the velocity of the second sound coincides with $v_0$, which allows us to conclude that a high-temperature second sound occurs primarily due to heat transfer by optical bending phonons.

VII. COMPARISON WITH CLASSICAL MOLECULAR DYNAMICS

Our simulation of the dynamics of temperature impulses and relaxation of periodic temperature lattices has shown that by using semi-quantum molecular dynamic, i.e., by taking into account the quantum statistics of thermal phonons, at a temperature of $T = 100\text{K}$ and below, a hydrodynamic heat transfer regime, the indicator of which is the second sound, is observed in carbon nanotubes and nanoribbons. The increase in temperature leads to a transition from the hydrodynamic to the diffusion regime of heat transfer. At room temperature $T = 300\text{K}$, there is no second sound. This conclusion is in agreement with the results of the experimental work [16], in which fast, transient measurements of the thermal lattices showed the existence of a second sound in graphite at temperatures of $85 < T < 125\text{K}$. To assess the importance of taking into account the quantum statistics of thermal phonons, we will check the existence of a second sound using the classical method of molecular dynamics, in which all phonons, regardless of temperature and their frequency, are equally thermalized.

In the classical method of molecular dynamics, to obtain a thermalized initial state of CNT (CLR) (31), it is necessary to integrate a system of Langevin equations with white noise (13), (14) with a temperature distribution (30) to simulate the motion of the temperature impulse, and with a distribution (32) to simulate the relaxation of the temperature lattice. The simulation of the motion of the temperature impulse has shown that with the same thermalization of all phonons, the wave-like motion of temperature in CNT and CNR does not occur even at low temperatures – see Fig. 14. For example, at $T = 50, 100\text{K}$, the transfer of the temperature impulse along the nanotube occurs in the form of its slow diffusion expansion, which is sharply different from the scenario obtained using the semi-quantum method – see Fig. 7. Modeling of the relaxation of the temperature lattice also shows that when using the classical method of molecular dynamics (with full thermalization of all phonons), temperature waves are not formed even at low temperatures, there is only a slow diffusion spreading of the temperature lattice – see Fig. 15. Thus, the classical molecular dynamics does not allow to simulate temperature waves experimentally observed in graphite [16, 17]. Therefore, it is fundamentally important to take into account the quantum statistics of thermal phonons for modeling the second sound in quasi-one-dimensional and two-dimensional molecular systems.

Note that graphene has a very high Debye temperature

![Graph with temperature profile](image1)

**FIG. 12:** Evolution of the relaxation temperature profile in the CNT (6,6) (length $N = 2^{13}$) for period $Z = 2^{l+1}$ ($l = 0, 1, \ldots, 7$) for (a) temperature $T = 100\text{K}$ ($\Delta T = 50\text{K}$) and (b) $T = 300\text{K}$ ($\Delta T = 150\text{K}$). Time dependence of the mode maximum $T(1)$ [blue lines] and minimum $T(1 + Z/2)$ [red lines] are depicted. Time scales are differ for each curve in order to fit them into one figure, time $t_0 = 0.04\text{ps}$.

![Graph with wave velocity vs. length](image2)

**FIG. 13:** Dispersion of thermal periodic waves for $T = 100\text{K}$. Dependence of the wave velocity $v$ on its length $L = aZ$ for both CNT and CNR (curves 1 and 2). Dashed lines mark the maximum values of the group velocities of the optical bending phonons of CNT ($v_o = 6.54\text{ km/s}$) and CNR ($v_o = 5.87\text{ km/s}$), respectively.

![Graph with Debye temperature](image3)
FIG. 14: Dynamics of the temperature pulse along CNT (6,6) at its initial temperature $T_h = 3T$, length $N_t = 40$ and background temperature (a) $T = 50K$ and (b) $T = 100K$. The dependence of the temperature distribution along CNT $T_n$ on the time $t$ is shown. The initial state of the temperature lattice is obtained using the classical approximation (with full thermalization of all phonons). The dashed (red) lines show trajectories for moving at a constant speed $v = v_o, v_t$ and $v_l$.

$T_D = \hbar \omega_m/k_B = 2300K$, where $\omega_m = 1600 \text{ cm}^{-1}$ is the maximum frequency of the phonon spectrum. Therefore, without taking into account the quantum statistics of phonons, it is impossible to obtain reliable results for graphene nanoribbons and nanotubes.

VIII. CONCLUDING REMARKS

Our numerical studies of heat transport in low-dimensional carbon structures has revealed that, in order to explain the observation of high-temperature second sound in crystalline graphite, it is critically important to taking into account quantum statistics of thermal phonons. In contrast, the classical method of molecular dynamics with full thermalization of all phonons does not allow simulating correctly second sound at temperatures $85 \div 125K$ observed in experiment [16]. When the quantum statistics is taken into account, only nonzero phonons with the average energy $k_B T p(\omega, T)$, where the density distribution of energy phonons $p$ depends on the temperature according to the formula (12), can participate in heat transport. By decreasing the temperature, only low-frequency phonons with frequencies $\omega < k_B T/\hbar$ remain fully thermalized.

From the form of the dispersion curves for nanoribbons and nanotubes (see Figs. 4 and 5), it follows that at $T = 300K$, almost all phonons with frequencies $\omega < 300 \text{ cm}^{-1}$ remain thermalized and participate in heat transfer. For low temperatures $T < 50K$, only low-frequency long-wave phonons participate in heat transfer. For a nanotube, these are two acoustic branches (longitudinal and torsional acoustic phonons having velocity $v_l$ and $v_t$) and two optical branches leaving the zero point (with wave number $q \searrow 0$, their phase velocity tends to zero). Therefore, for very low temperatures, acoustic long-wave phonons make the main contribution to heat transfer, thus defining the ballistic regime of heat transfer. For high temperatures, the participation of all phonons in heat transfer leads to a diffusion regime. For
intermediate temperatures 50–150K, only low-frequency phonons participate in heat transfer, a large part of them will be accounted for by bending phonons – see Fig. 4(b).

For a nanotube, optical bending waves have a maximum group velocity \( v_g = 6.54 \text{ km/s} \) – the velocity of bending phonons with dimensionless wave numbers \( q \approx [0.05, 0.5] \) (see Fig. 5). For a nanoribbon, this velocity is \( v_g = 5.87 \text{ km/s} \). For temperatures 50–150K, bending phonons with these wave numbers make the main contribution to heat transfer. In the simulations, the motion of these phonons appears as the motion of a temperature maximum at velocity \( v = v_0 \) – see Figs. 6 and 7. Therefore, we can conclude that second sound observed in graphite at liquid nitrogen temperatures corresponds primarily to the motion of optical bending vibrations.

Second sound will be absent for very low temperatures \( T < 20\text{K} \), since in this case bending phonons with velocities close to \( v_0 \) will no longer participate in heat transfer. For high temperatures \( T > 200\text{K} \), second sound becomes faintly noticeable, since many phonons here already participate in heat transfer, and the contribution from the motion of low-frequency bending phonons will remain relatively small.

Thus, we come to the conclusion that, for carbon nanoribbons and nanotubes, high-temperature second sound is caused by low-frequency bending phonons. The existence of such phonons follows from the one-dimensionality or two-dimensionality of the molecular systems. Therefore, we should expect second sound in such two-dimensional systems as graphene (graphite) [16, 17], hexagonal boron nitride (h-BN), and in quasi-one-dimensional systems such as graphene and h-BN nanotubes, linear cumulene macromolecule [44], and planar zigzag polyethylene. In quasi-one-dimensional systems, second sound manifests itself more strongly than in quasi-two-dimensional systems, since bending vibrations of the former make a greater contribution to heat transfer. The speed of second sound in such molecular structures can be estimated as the maximum group velocity of bending optical phonons whose dispersion curve split off the zero point. Our results suggest that the velocity of second sound in graphene (graphite) is about 6 km/s.

Finally, we notice that, because bending vibrations have nonzero dispersion [45, 46], there are no optical bending phonons in two-dimensional layers of MoS\(_2\), MoSe\(_2\), WS\(_2\), and WSe\(_2\) where the molecular layers have a finite thickness (such as flat corrugated structures). Therefore, high-temperature second sound should not be observed in all such structures. Instead, only a ballistic regime should be expected, with a transition to a diffusive heat transfer regime with a growth of temperature.

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