NANOSYSTEMS:
PHYSICS, CHEMISTRY, MATHEMATICS

Rudyak V.Ya., Lezhnev E.V. *Nanosystems: Phys. Chem. Math.*, 2023, **14** (2), 186–194.
http://nanojournal.ifmo.ru
DOI 10.17586/2220-8054-2023-14-2-186-194

Original article

Modeling the rarefied gas thermal conductivity in nanochannels

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PACS 51.20.+d, 02.70.Ns

ABSTRACT In the paper, the thermal conductivity of rarefied gases in nanochannels and in bulk was studied. The following gases Ar, Kr, Ne, Xe, O_2, CH_4 were considered. The evolution of gas molecules in phase space was calculated by the method of the stochastic molecular modelling. It was established that the thermal conductivity coefficient of the gas in the nanochannel is anisotropic. Anisotropy of the thermal conductivity is caused by the interaction of gas molecules with the channel walls. This interaction is described by the specular or diffuse laws of molecules reflection. The thermal conductivity of gases across the channel is significantly lower than along it. The anisotropy of the thermal conductivity persists even in microchannels, but it decreases with the increasing of the gas density. In fact, the thermal conductivity coefficient is not a gas property only, but of a gas+channel wall system.

KEYWORDS nanochannel, rarefied gas, stochastic molecular simulation, thermal conductivity, transport processes.

ACKNOWLEDGEMENTS This paper was supported partly by the Mega-Grant from the Ministry of Science and Higher Education of the Russian Federation (Agreement no. 075-15-2021-575).

FOR CITATION Rudyak V.Ya., Lezhnev E.V. Modeling the rarefied gas thermal conductivity in nanochannels. *Nanosystems: Phys. Chem. Math.*, 2023, **14** (2), 186–194.

1. Introduction

In the last two decades, various devices and systems where flows in nanochannels take place have been rapidly developing. First of all, we can mention various biomedical systems, NEMS systems, nanomixers, etc. [1–5]. Thermophysical applications of nanoflows are of a great interest also, for example, thermoelectric energy conversion, thermal management of nanoscale electronics, creation of a chip-level cooling system, etc. For obvious reasons, the experimental study of heat transfer in nanochannels and the measurement of the thermal conductivity coefficient is extremely difficult. An alternative method for studying these properties is the molecular dynamics one. Thermal conductivity of liquid argon in plane channels with krypton walls was studied [6]. The channel height did not exceed 6 nm. It was found that the coefficient of thermal conductivity is slightly lower than in the bulk in small channels (2–3 nm high), but then it grows and reaches a value in the bulk.

Thermal conductivity of liquid argon in nanochannels was calculated in a wide range of fluid densities in paper [7]. The transverse size of the nanochannel varied from 2.25 to 15 nm. It was shown that the thermal conductivity weakly depends on the shape (square or round) of the nanochannel with the same cross-sectional area and it increases with the growth of the transverse size of the channel. In addition, the thermal conductivity coefficient reached values in the bulk for a certain characteristic channel size, which strongly depended on the fluid density and varied from 5 to 11 nm. Here, however, it should be noted that the interaction of argon molecules with the walls was described by a rather rough potential (power-law repulsion with an exponent equal to 96).

Pourali and Maghari [8] simulated the thermal conductivity of a binary mixture of methane and some n-alctanes in a fairly narrow channel using the nonequilibrium molecular dynamics method. In order to create a temperature gradient, the walls of a plane channel had different temperatures. It was indicated that the thermal conductivity of the mixture increased with the decreasing of the channel height.

In the recent paper [9], a significant anisotropy of thermal conductivity along and across channel was established. This also agrees with experimental data [10]. The presence of such anisotropy is a natural consequence, firstly, of anisotropy of the channel geometry, and, secondly, of a great influence of fluid molecules interaction with the channel walls.

It was shown [11, 12] by methods of nonequilibrium statistical mechanics that, under confined conditions, the constitutive relations are transformed. In particular, a contribution appears in the transport coefficients due to the interaction of fluid molecules with the channel walls. Thus, in particular, it was found that the fluid viscosity is a property of the entire fluid+channel wall system. Therefore, by varying the material of the walls, the viscosity can be controlled, it can be either more than in the bulk or less [13].

Finally, we should mention paper [14], where the thermal conductivity of water in a plane nanochannel with graphene walls was studied by the method of molecular dynamics. The maximum channel height was about 15 nm. Anisotropy of thermal conductivity was also established there. The degree of this anisotropy decreased with increasing of the channel height.

In all the papers cited above, thermal conductivity of liquids was studied by the method of molecular dynamics. However, from a practical point of view, data on the thermal conductivity of rarefied gases in nanochannels are also necessary. In this case, the molecular dynamics method is not actually applicable, since it requires the use of a huge number of molecules (characteristic size of the simulation cell must be greater than the mean free path of gas molecules). A special algorithm was developed [15] called the smart wall molecular dynamics (SWMD) to reduce the required calculation time. Later, this method was used to solve a number of problems of rarefied gas dynamics in nanochannels [16–18]. In the last work, heat transfer of argon in a plane nanochannel 5.4 nm high was studied. The great importance of gas molecules interaction with the channel walls was noted.

The problem of heat transfer of rarefied gas in nanochannels continuously attracts attention of many researchers and many attempts have been made to solve it [19–21], but it has not been established yet, whether there is a difference between the thermal conductivity coefficient of rarefied gas in nanochannels and the corresponding values in the bulk. The study of the thermal conductivity coefficient of a rarefied gas in confined conditions is an important factor in solving many practical problems. The influence of gas rarefaction degree on the coefficient is known, however, rigorous formulas can be obtained in the case of small or, on the contrary, large (in free molecular limit) Knudsen numbers. In the last case, a semi-phenomenological formula was actually obtained, where the thermal conductivity coefficient depended on the so-called accommodation coefficients, which described the interaction of gas molecules with the channel walls. In this connection, an attempt to calculate the accommodation coefficients of argon in channels with platinum walls using the molecular dynamics method was made [22]. One can see that these coefficients increase with decreasing temperature and tend to unity. Nevertheless, it should be noted that with this approach it is not possible to understand how the anisotropy of the transport processes affects the effective coefficient of thermal conductivity.

Previously, the authors developed the method of stochastic molecular modeling (SMM) for simulation of the transport coefficients of rarefied gases [23–26]. This method has been used to simulate the coefficients of self-diffusion, diffusion and viscosity of various gases, including polyatomic and rarefied gas nanosuspensions with high accuracy [26] (with the accuracy of experimental measurements). The viscosity of rarefied gases in nanochannels was also studied [27] and its anisotropy was established. The purpose of this paper is to calculate the thermal conductivity coefficients of rarefied gases in nanochannels using SMM method. Thermal conductivity of argon, krypton, xenon, oxygen, and methane in nanochannels with a square cross section was studied, and the channel height varied from 8.5 to 1000 nm. The coefficient of thermal conductivity in the bulk was also preliminarily calculated, which value was compared with the known experimental data. The accuracy of such modeling is also discussed.

2. Algorithm of the SMM Method

In this paper, we are talking about modelling the thermal conductivity coefficient of rarefied gases in nanochannels. Usually, the transport coefficients of rarefied gases are calculated using the kinetic theory of gases. One of the main achievements of this theory is derivation of formulas for calculating these coefficients (see, for example [28, 29]). Their calculation, however, in the general case is not an easy task and requires implementation of many time-consuming procedures, in particular, solution of fairly complex integral equations. Nonequilibrium statistical mechanics makes it possible to construct universal generalized constitutive relations and deduce explicit formulas for the transport coefficients [30–32]. In this case, the transport coefficients are determined by the so-called fluctuation-dissipation theorems (FDTs). In the literature they are usually called Green–Kubo formulas. According to FDTs, the transport coefficients are time integrals of two-time correlation functions of the corresponding dynamic variables. The equivalence of the formulas for the transport coefficients of the kinetic theory of gases to the Green–Kubo formulas is proved [33, 34]. In particular, the thermal conductivity coefficient λ is determined by the formula:

$$\lambda = \frac{k}{3VT^2}\int\limits_0^{\tau_p} \langle \mathbf{j}(0)\cdot\mathbf{j}(t)\rangle dt = \frac{k}{3VT^2}\int\limits_0^{\tau_p} \chi(0,t)dt, \tag{1}$$

where k is Boltzmann's constant, V is system volume, $\mathbf{j}$ is microscopic vector of heat flux, τ_p is the so-called plateau value of the integration time. Actually, an experimentally measurable value of the transport coefficient is obtained by reaching this value [35]. During this time, the corresponding autocorrelation function of thermal conductivity (TCACF) $\chi(0,t)$ damps. The angle brackets in (1) mean ensemble averaging. It is important to emphasize that the averaging in (1) is carried out over the equilibrium ensemble, and the transport coefficients and thermal conductivity coefficient, in particular, are determined by the properties of thermal equilibrium molecular fluctuations. This also corresponds to the kinetic theory of rarefied gases, where the transport coefficients are calculated by the Maxwell distribution function [28, 29].

The calculation of correlation functions requires information about the dynamic variables of the system being modeled at successive moments of time. In a rarefied gas, the interaction of molecules does not contribute to the transport coefficients and to the equation of state. The corresponding contributions appear only in the so-called nonideal gas [36,37]. For this reason, to model the transport coefficients of a rarefied gas, it is sufficient to have data on its dynamic variables only in the velocity space. Therefore, the microscopic vector of the heat flux in formula (1) depends only on the velocities of the molecules. In confined conditions and in nanochannels, in particular, there is an intense interaction of gas molecules with the channel walls. This leads to the fluctuation motion of the center of mass of the considered equilibrium gas (the average velocity of the gas center of mass is equal to zero, of course). This fluctuation motion changes the energy transfer in the system, and this contribution should be excluded to calculate the true thermal conductivity of gas. Therefore, the microscopic vector of the heat flux of a rarefied gas in confined conditions is described by the following relation:

$$\mathbf{j}(t) = \sum_{i}^{N} [\mathbf{v}_i(t) - \mathbf{v}_c(t)] e_i(t), \quad \mathbf{v}_c(t) = \frac{1}{N} \sum_{i}^{N} \mathbf{v}_i(t), \tag{2}$$

where $\mathbf{v}_c$, $\mathbf{v}_i$ and e_i are, respectively, the velocity of the mass center, the velocity of the molecule i and its kinetic energy, and N is the number of molecules in the system.

Below, the contribution due to the energy transfer associated with fluctuations in the velocity of the center of mass of gas will be called the fluctuation contribution. Calculating the thermal conductivity coefficient, the velocity of the center of mass, of course, is equal to zero in the bulk.

So, in order to calculate TCACF and, consequently, the thermal conductivity coefficient, it is necessary to have data on all molecules velocities of the simulated system at successive moments of time. In confined conditions, in addition to the interaction of gas molecules with each other, they also interact with the channel walls. For this reason, SMM algorithm became more complicated, since information about the coordinates of all molecules was also required at each moment of time. The interaction of gas molecules with the channel walls is described in this work using specular or specular-diffuse reflection law. This approach is typical for rarefied gas dynamics [38, 39]. In specular reflection, the velocity of a molecule along surface does not change, but its normal component changes its sign. In diffuse mode, the velocity of the reflected molecule is played out according to the Maxwell distribution function. In specular-diffuse reflection, the fraction of molecules θ interacts with the wall diffusely, while $(1-\theta)$ interacts specularly, where θ is the so-called accommodation coefficient. The molecules interaction is described by Lennard-Jones potential:

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right], \tag{3}$$

where σ and ε are the effective molecular size and the potential well depth, respectively.

The simulation cell is chosen in the form of a parallelepiped with a square cross section, along its axis periodic boundary conditions are set, which are usual for the method of molecular dynamics [40]. In accordance with the given mass density of gas ρ (or numerical one), the molecules are distributed uniformly over the simulation volume. Their velocities are played out according to the Maxwell distribution with a given temperature, but in such a way the total momentum of all N molecules is equal to zero (the corresponding procedure is described in [25]), since the equilibrium state of gas is simulated. Simulating the dynamics of gas in question begins with listing. At the initial time t, all molecules are listed in some arbitrary order. By changing the order of the particles in the list, we will get different phase trajectories. Thus, at time t, the particles have velocities $\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_N$ and coordinates $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N$.

In order to obtain the values of dynamic variables at successive time moments, their dynamics is split into processes, and the motion of molecules in the space of velocities and configurations is successively modeled. The phase trajectory calculation time t_s is divided into intervals of duration $\tau_\alpha = \sigma/v_\alpha(t)$ where σ is the effective molecular diameter, and v_α is the maximum velocities of the system molecules at a given time. The formation of the list at the first-time step $(t+\tau_1)$ begins with the consideration of molecule 1. First, the coordinate of this molecule is changed, $\mathbf{r}(t+\tau_1) = \mathbf{r}_1(t) + \mathbf{v}_1(t)\tau_1$, and its collision with the wall is checked. If the interaction with the wall has occurred, then the molecule velocity changes depending on the law of interaction with the wall used in this calculation (specular, diffuse or specular-diffuse) and the coordinate changes accordingly. If there is no interaction with the wall, then its collision with other gas molecules is played out. For this purpose, a random number u is generated, uniformly distributed over the interval (0;1). If it turns out to be less than or equal to the average collision probability [29] $P_{c1} = 4\tau_1 \rho \sigma^2 \sqrt{\pi RT/m}$, then a collision will occur. In this case, molecule j is randomly selected from the remaining $(N-1)$ molecules, with which the collision is realized. As a result, the molecules velocities 1 and j change in accordance with the conservation laws. If the played number u turns out to be greater than the average collision probability, then molecule 1 does not collide and its velocity does not change. This is how all molecules are sequentially processed and a complete list of dynamic variables at the moment $(t+\tau_1)$ is formed. After that, the next time interval $\tau_2 = \sigma/\mathrm{v}_\alpha(t+\tau_1)$ is selected, and the procedure is repeated. Then the same procedure is implemented for each time step until the specified calculation time t_s is over. Thus, a complete set of dynamic variables of all simulated system's molecules is obtained at successive time moments.

TABLE 1. Comparison of calculation data for the thermal conductivity coefficient of rarefied gases by SMM method λ with experimental [41] λ_e $\mathrm{Wm^{-1}K^{-1}}$

	Ar	Kr	Ne	Xe	O_2	CH_4
λ	0.0175	0.0098	0.0506	0.0055	0.0279	0.0329
λ_e	0.0177	0.0096	0.049	0.0057	0.0267	0.0342
Δ %	1.23	2.52	3.36	3.17	4.49	3.93

3. Thermal Conductivity of Rarefied Gas in the Bulk

Modeling gas thermal conductivity in a nanochannel requires, first of all, SMM method verification, which is used for this purpose. On the one hand, it is necessary to verify this method, calculating the transport coefficients in the bulk, and on the other hand, in nanochannels themselves. Previously [23–26], the efficiency and accuracy of SMM method were demonstrated, calculating the coefficients of self-diffusion, diffusion, and viscosity of rarefied gases, including polyatomic gases. In all cases, it is possible to achieve an accuracy of 1–2% using a relatively small number of molecules. The accuracy grows with an increase in the number of molecules used for modeling and phase trajectories over which the calculated data are averaged. There are no experimental data on measuring gases thermal conductivity in nanochannels. However, it is clear from physical considerations that the coefficient of gas thermal conductivity along a sufficiently long channel should be consistent with its value in the bulk (unless the channel is too narrow). Therefore, SMM method verification in this case consists of two parts, the thermal conductivity coefficients of rarefied gases in the bulk and along nanochannel are calculated.

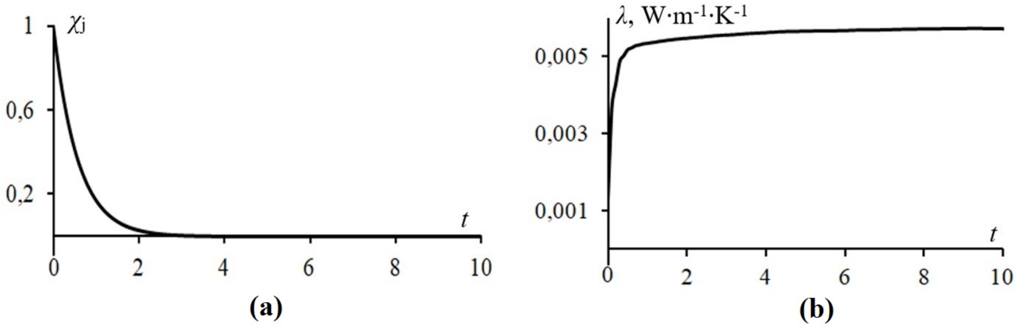

FIG. 1. Evolution of a) TCACF and b) thermal conductivity coefficient (1)

The calculation of the thermal conductivity of rarefied gases is still a rather complex problem in the kinetic theory of rarefied gases. If the first approximation of expansion in terms of Sonin polynomials is usually sufficient to calculate the diffusion and viscosity coefficients, then this is not the case for thermal conductivity. Therefore, direct numerical simulation of thermal conductivity is really relevant. Previously, such modeling was not performed by SMM method. This has been done for the first time below. Both monatomic (Ar, Kr, Ne, Xe) and polyatomic gases (CH_4, O_2) were considered. The thermal conductivity coefficient was calculated using FDT (1), but the velocity of the gas mass' center should be set equal to zero, calculating the correlation function (see formula (2)). Since gas is rarefied, TCACF χ should decay exponentially, which is shown by the calculation data presented in Fig. 1a. Here the calculation of the xenon TCACF is presented, the time is normalized to the mean free path time of the molecule. Indeed, over the time order of several free path times of molecules, TCACF relaxes. Exponential damping of the correlation function means a rather fast reaching of the plateau value of the corresponding transport coefficient, i.e., the thermal conductivity coefficient. Figure 1b illustrates this evolution.

Systematic data obtained for all the above gases are given in Table 1. All calculations were performed at atmospheric pressure and a temperature of 300 K. 3200 molecules were used, averaging was carried out over 1000 independent phase trajectories. The calculation data turn out to be quite comparable with the experimental ones. For argon, krypton, and xenon, they were obtained within the measurement accuracy (Δ is relative error), which is usually 2–3%. For the three remaining gases, the accuracy is slightly worse.

The accuracy of any molecular modeling, including SMM method, depends on several factors. First of all, it depends on the choice of the molecular interaction potential used. Strictly speaking, it is impossible to formulate universal recipes for their choice. Everything depends on the problem being solved. Situation is somewhat simplified, calculating the integral characteristics of fluids. Here we can choose rather simple potentials. However, success is largely determined by the choice of potential parameters. This should be treated very carefully. For example, it is difficult to expect high accuracy of viscosity modeling, determining the parameters of the potential from diffusion data. Nevertheless, it can be stated that SMM method is quite conservative with respect to such a choice. High accuracy can be obtained even using the known parameters of Lennard-Jones potential, which are obtained from a variety of experimental data.

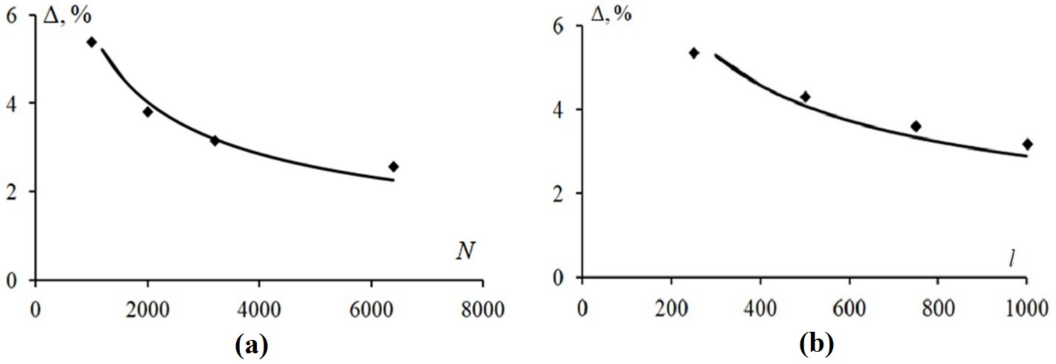

FIG. 2. Dependence of the relative error Δ for calculating the thermal conductivity coefficient of xenon on a) the number of molecules used and b) the number of trajectories

The calculation accuracy is affected both by the number of molecules used and by the number of independent trajectories over which the averaging is carried out. In this paper, the influence of both these factors is systematically studied. As an example, Figure 2a shows the dependence of the calculated values of xenon thermal conductivity on the number of molecules. 750, 1500, 3000 and 6400 molecules were used in the calculations; the calculated data in Fig. 2 correspond to the rhombuses. The calculation error Δ with an increase in the number of molecules systematically decreases and is well (the correlation coefficient is 0.97) described by the dependence: $\Delta = 175.17/\sqrt{N}$, which corresponds to a continuous curve in Fig. 2a. High accuracy in calculating the thermal conductivity coefficient can also be obtained for polyatomic molecules. For example, when 6400 molecules are used in calculations, the error in determining the thermal conductivity coefficient of oxygen is 0.93%, and that of methane is 0.67% (averaging was carried out over 1000 phase trajectories).

The second important circumstance that determines the accuracy and time of the calculation is the number of ensemble members (the number of independent phase trajectories) over which the obtained data are averaged. The ensemble, over which the averaging is carried out, is a typical Gibbs ensemble characterized by different initial phase states of molecules for given average values of macroscopic observables. The accuracy of modeling the thermal conductivity coefficient also increases with an increase in the number of ensemble members. Figure 2b shows the dependence of the relative error obtained, calculating xenon thermal conductivity. Here, the number of molecules used was 3000, and the number of trajectories varied from 250 to 1000 (the rhombuses). Together with an increase in the number of phase trajectories, the relative errors decrease monotonically and are well described by the dependence: $\Delta_1 = 91.29/\sqrt{L}$ (the correlation coefficient is 0.98). It is necessary to use about 8000 trajectories to obtain accuracy of the order of a percent, using 3000 molecules.

4. Thermal Conductivity of Gas in Nanochannels

In present paper, the thermal conductivity of argon, krypton, xenon, oxygen, and methane in nanochannels with a square cross section is studied, the channel height is varied from 8.5 to 1000 nm. The thermal conductivity coefficient was calculated using FDT (1). As it is already mentioned, there is a significant movement of the center of mass in the gas. In fact, some specific two-phase medium takes place. In order to calculate true gas thermal conductivity, the contribution due to the fluctuation motion of the mass center of gas should be excluded. In what follows, the contribution associated with energy transfer due to fluctuations in the velocity of the mass center of gas will be called the fluctuation contribution. The calculations were performed at a pressure from one to ten atmospheres and a temperature of 300 K.

First of all, it should be noted that with both the specular and diffuse laws of interaction of gas molecules with the walls, a significant anisotropy of thermal conductivity is recorded along and across the channel, the thermal conductivity across the channel is extremely low. As an example, Fig. 3a shows the dependence of the thermal conductivity coefficient along the channel with a fluctuation contribution (square marks) and without it (round marks) at atmospheric pressure in a channel with specular walls. The dotted line corresponds to the value of the thermal conductivity coefficient in the bulk. It should be noted that in the nanochannels presented here, the coefficient of longitudinal thermal conductivity (along the channel) is higher than in the bulk, although this excess is small. As the channel height increases, thermal conductivity along it tends to the thermal conductivity in the bulk. The coefficient of thermal conductivity in the bulk under these conditions is equal [42] to 0.01767 $\mathrm{Wm^{-1}K^{-1}}$. The difference in the thermal conductivity coefficient without fluctuation contribution along the channel at its height equal to 35 nm from the corresponding value in the bulk is already less than 1%. Thus, SMM method quite adequately predicts its value. It should be highlighted, however, that the accuracy of modeling the thermal conductivity along a channel also depends on its length, despite the fact that periodic boundary conditions are used along it. In this case, this length is 100 nm.

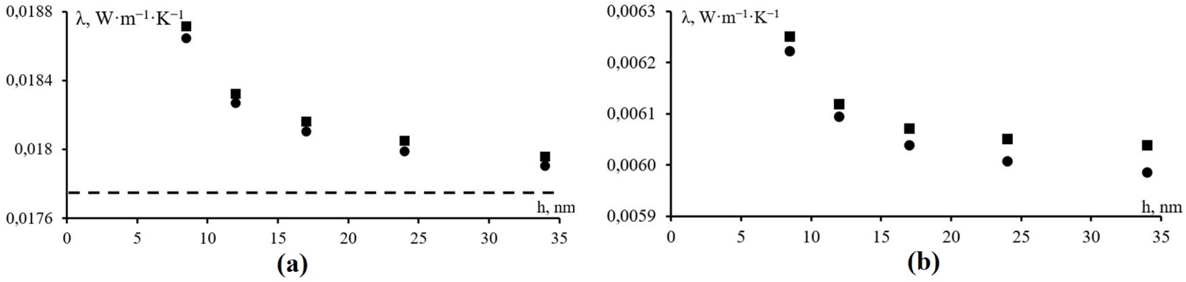

FIG. 3. Dependence of a) longitudinal and b) total thermal conductivity taking into account fluctuation contribution (square marks) and without it (round marks) on the channel height

The anisotropy of the thermal conductivity in a nanochannel is very large. The thermal conductivity coefficient across the channel (there are two such directions) in this case turns out to be three orders of magnitude smaller than the value fixed in the bulk. As a result, the total thermal conductivity coefficient is almost three times less than in volume. This is illustrated in Fig. 3b, which shows the dependence of the total thermal conductivity coefficient on the height of nanochannel. Here again, round marks correspond to the total thermal conductivity without a fluctuation contribution, and square marks correspond to a fluctuation one.

Two circumstances should be noted. First, the coefficient of thermal conductivity in the channels of minimum cross section is only a third of the corresponding value in the bulk, and then increases. However, the total thermal conductivity is almost two and a half times less than in the bulk even in a channel with a height of 35 nm. This means that although anisotropy weakens with increasing channel size, thermal conductivity across the channel is still quite low. The anisotropy is also preserved in sufficiently large channels. As a consequence, the total thermal conductivity in a nanochannel 500 nm high is slightly more than half of the value in the bulk (see Fig. 4). However, even in a channel with a height of 1 μm, thermal conductivity in the channel is approximately 40% lower than in the bulk (see Fig. 4).

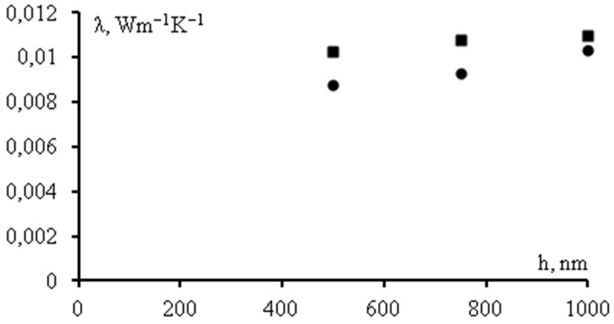

FIG. 4. Dependence of the total thermal conductivity with fluctuation contribution (square marks) and without it (round marks) at 300 K and atmospheric pressure from the channel height

The second aspect to note is the fluctuation component contribution, which somewhat increases with increasing channel cross section, although this contribution barely exceeds 1% in a channel with a height of $h = 35$ nm. Then it reaches maximum; at $h = 500$ nm, it is almost 17% here, but decreases with a further increase in the channel cross section: at $h = 750$ nm, it decreases to 15.7%, and at $h = 1$ μm, to 5.9%. It should also be kept in mind that the fluctuation contribution is especially large to the thermal conductivity across the channel. This contribution is especially noticeable in channels with a small cross section. For example, in a channel with a height of 35 nm, it is 183.4%. On the other hand, in a channel with a height of 1 μm, this contribution decreases to 13.5%.

So far, we have been talking about channels with specular walls. The character of the molecules interactions with walls significantly affects thermal conductivity, although the main qualitative characteristics remain unchanged. The dependence of the total thermal conductivity with fluctuation contribution λ_t and without it λ in a channel with diffuse walls on the channel height is presented in Table 2. Here again, gas temperature is 300 K. The last line shows relative difference between these two values of thermal conductivity. Thermal conductivity in a channel with diffuse walls is less than in the bulk and increases monotonically with increasing channel height. This applies to both longitudinal and transverse components. However, it remains 3 times less than in the bulk even in a channel with a height of 1000 nm. Such a low value of the thermal conductivity coefficient even in a channel with a height of 1 micron is associated with significant anisotropy of thermal conductivity. The thermal conductivity coefficient across the channel increases with

TABLE 2. Dependence of the total thermal conductivity with fluctuation contribution λt and without it λ in a channel with diffuse walls on the channel height

h, nm	8.5	17	34	500	750	1000
λ_t, W·m^{-1}·K^{-1}	9.22·10^{-5}	2.54·10^{-4}	7.56·10^{-4}	0.00278	0.00328	0.00517
λ, W·m^{-1}·K^{-1}	7.97·10^{-5}	2.32·10^{-4}	7.16·10^{-4}	0.00274	0.00324	0.00511
Δ, %	15.68	9.58	5.68	1.38	1.35	1.10

TABLE 3. The thermal conductivity coefficient with fluctuation contribution λ_t and without it λ in a channel with specular walls 500 nm high at a pressure of 10 atm

	λ_t, W·m^{-1}·K^{-1}	λ, W·m^{-1}·K^{-1}	Δ, %
OX	0.0146	0.0139	5
OY	0.0182	0.0181	0.5
OZ	0.0146	0.0139	5
λ_a, W·m^{-1}·K^{-1}	0.0158	0.0153	3

increasing channel height. If the transverse coefficient was 800 times less than in the bulk at a channel height of 8.5 nm, then it is only 8 times less than in the bulk at a channel height of 1000 nm.

It is important to emphasize that, thermal conductivity along the channel is close to thermal conductivity in the bulk (even somewhat exceeds it in channels of low height) under the specular law of interaction. On the contrary, in channels with a diffuse law of molecule interaction with walls in small channels, the longitudinal coefficient of thermal conductivity is always lower than in volume. In a channel with a height of 8.5 nm, it is less than in the bulk by about 80 times, and in a channel with a height of 1 μm, by 1.5 times.

In conclusion, we present the data of modeling the thermal conductivity coefficient by the SMM method at a temperature of 300 K and a pressure of 10 atm. A channel with specular walls 500 nm high was considered. This corresponds to Knudsen number Kn = 0.014. The thermal conductivity coefficient in the bulk in this case is [42] 0.01809. Simulation data are given in Table 3. Here, the longitudinal coefficient of thermal conductivity corresponds to OY axis, the other two are transverse. The bottom line shows the total coefficient of thermal conductivity, which is, in fact, the average in all three directions. In the last column, one can see the relative difference between thermal conductivity with and without the fluctuation contribution. The analysis of the table shows that the anisotropy of thermal conductivity is also preserved here, although it is significantly lower than at atmospheric pressure. The total thermal conductivity is only 3% lower than in bulk. In this case, the longitudinal coefficient of thermal conductivity practically coincides with the bulk value. Contribution of heat transfer caused by fluctuations in the velocity of the mass center of the system is almost absent in longitudinal direction and only 5% in transverse one.

5. Conclusion

In present paper, the thermal conductivity of rarefied gas in nanochannels has been studied. First, it is necessary to note its anisotropy. Previously, such anisotropy has already been observed in nanochannels with liquid [6–10]. In the case of rarefied gas, this anisotropy is much higher. As it is shown above, the thermal conductivity coefficients along and across the channel can differ by three orders of magnitude. As the channel height increases, the degree of anisotropy decreases, but it turns out to be significant even in microchannels. On the other hand, the rarefied gas thermal conductivity along the channel is consistent with the corresponding values in the bulk (if the channel is long enough). Finally, it should be noted that with an increase in gas density (pressure), the degree of anisotropy of thermal conductivity decreases.

The total (average) thermal conductivity value of a fluid in a nanochannel depends significantly on the interaction of its molecules with the channel walls. In fact, the thermal conductivity coefficient is not a gas property only, but of gas+channel wall system. For this reason, it is possible to change the effective coefficient of thermal conductivity by varying the walls' material, and hence heat transfer in nano and microchannels.

There is another important aspect. Fluid in nanochannels is some specific two-phase system. There is a fluctuation contribution to the thermal conductivity coefficient due to the presence of fluctuations in the velocity of the center of mass in equilibrium gas. It is clear that this contribution decreases with increasing channel height. This is confirmed by the performed calculations. However, this contribution still takes place even in microchannels. It should be understood that in real nanodevices, heat transfer will be determined by the total thermal conductivity coefficient, taking into account the fluctuation component. In this sense, fluctuation contribution in nanochannels is somewhat analogous to convective heat conduction. Therefore, if there is a flow in the nanochannel, then along with the fluctuation component of thermal conductivity, there is also a convective one. Moreover, the convective component can be much larger than the fluctuation one.

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Submitted 2 March 2023; accepted 16 March 2023

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Conflict of interest: the authors declare no conflict of interest.