Low-Temperature Heat Transfer in Nanowires

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A new regime of low-temperature heat transfer in suspended nanowires is predicted. It takes place when (i) only "acoustic" phonon modes of the wire are thermally populated and (ii) phonons are subject to the effective elastic scattering. Qualitatively, the main peculiarities of heat transfer originate due to the appearance of the flexural modes with high density of states in the wire phonon spectrum. They give rise to the $T^{1/2}$ temperature dependence of the wire thermal conductance. Experimental situations where the new regime is likely to be detected are discussed.

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Most often, in dielectrics and semiconductors heat is conducted by means of phonon transfer. At low temperatures it is controlled by the phonon scattering at the surface of the sample, since the internal mechanisms of scattering due to the lattice anharmonicity and intrinsic defects provide the phonon mean free path far above the typical dimensions of the sample. In this case the phonon transfer is similar to the gas flow in small pipes in the Knudsen regime and, strictly speaking, it is impossible to introduce local Fourier law for determination of the heat flux density [1]. However, for the samples in the shape of a wire it is still possible to speak about the thermal conductance, σ_T, that is defined as a ratio of the heat flux through the wire and the temperature difference between the reservoirs connected by the wire. If phonon scattering at the surface is diffusive, then $\sigma_T \sim T^3$. Decrease of temperature, however, increases the characteristic phonon wavelength and reduces the scattering probability at the surface. If the probability of the specular phonon scattering at the surface is close to unity, then the phonon spectrum is substantially modified. For ideal wires having constant cross section it is broken in a set of branches where the phonon frequency ω depends on the 1D wave vector q directed along the wire axis [2,3]. In this Letter we consider heat transfer at extremely low temperatures. Speaking about the low temperatures, we mean that only the phonon states of the "acoustic" branches with $\omega \to 0$ at $q \to 0$ are thermally populated. In other words, we assume $T \ll \hbar\Delta\omega$, where $\Delta\omega$ is the characteristic value of the frequency gap between the adjacent phonon branches, $\Delta\omega \sim v/a$, where v and a are the characteristic sound velocity and dimension of the wire cross section, respectively. This condition corresponds to the effective reduction of the phonon momentum space dimensionality. It can be realized in the modern suspended films and wires, employed for the fundamental studies of the phonon confinement and electron-phonon interaction [4,5], and as elements of ultrasensitive phonon detectors [6]. Normally, condition $T \ll \hbar\Delta\omega$ corresponds to subkelvin temperatures. So, for $a = 100$ nm and $v = 5000$ m/s, $\hbar\Delta\omega$ corresponds to the temperature about 0.4 K. If the wire structure is perfect enough, then phonons are transferred between the reservoirs ballistically. Ballistic transfer in wires was studied theoretically in Refs. [7–9], where both thermal conductance and phonon correlation characteristics have been analyzed. It was found that in the ballistic regime each phonon branch can contribute to the value of the thermal conductance no more than the fundamental quantum $\pi T/6\hbar^4$, regardless of the phonon spectrum details. This prediction was recently confirmed experimentally [10]. In this Letter we consider the opposite case, when phonons are multiply scattered elastically while being transferred through the wire. A similar problem was analyzed previously in Refs. [11,12] where the numerical calculations of the phonon transmission through the imperfect wire have been performed. In these works, however, the authors used simplified models of the wire phonon spectrum and miss some qualitative features of heat transfer. We demonstrate in this Letter that for the case of effective phonon scattering at low temperatures the thermal conductance is proportional to $T^{1/2}$. This feature is qualitatively different from the ballistic phonon transfer and from the surface-scattering-controlled transfer of 3D phonons. We show that the main physical peculiarity of the 1D phonon transfer in wires is due to the special features of the wire phonon spectrum in the low-frequency region. Namely, some of the acoustic branches have quadratic dispersion and, therefore, high density of states and small group velocity. This substantially affects phonon scattering probabilities as well as the partial contributions of the phonons of a particular type to the heat flux. Note that similar effects arising due to the high density of states of the low-dimensional phonons for electron-phonon interaction in thin films have been reported recently [13]. In the experiments, the $\sigma_T \sim T^{1/2}$ dependence should replace $\sigma_T \sim T$, characteristic for the ballistic phonon transfer, with temperature increase. We show that the temperature interval where the considered regime of heat transfer can be detected grows with an increase of the phonon scattering and the length of the wire.

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As is well established [3], in free-standing wires there are four acoustic branches having the following dispersion at $qa \ll 1$:

$$\omega_{d,t} = v_{d,t} q, \qquad \omega_{f1,f2} = v_{f1,f2} a q^2. \tag{1}$$

Here d, t, $f1$, and $f2$ label the dilatational, torsional, and two flexural branches. The values of v_d, v_t, v_{f1}, and v_{f2} are of the order of the sound velocity. Their specific values are determined by the elastic properties of the wire material and by the shape of the wire cross section. To describe the steady-state heat transfer we use the standard kinetic equation for the phonon distribution function f:

$$\frac{\partial f_i}{\partial x} g_i = St_i\{f\}, \tag{2}$$

where $i = d, t, f1, f2$; g_i is the phonon group velocity, the x axis is directed along the wire, and $St\{f\}$ is the integral of collisions. Here we consider only elastic scattering of the phonons by the defects of the wire structure. These defects can be either due to the intrinsic imperfections of the crystal, say, natural isotopes, or can arise in the course of the nanowire fabrication process. Note that in actual suspended nanowires the latter source, in particular, surface roughness, is likely to provide the major contribution to the phonon scattering. We do not take into account three-phonon inelastic scattering due to the crystal anharmonicity. Having evaluated the corresponding phonon mean free path, we have found that it far exceeds the typical length of the wires, about tens of microns. Under this approach for $St\{f\}$ we have

$$St_i\{f\} = \sum_{j,q'} \{W^{(ji)}_{q'q} f_j(q')[1 + f_i(q)] - W^{(ij)}_{qq'} f_i(q)[1 + f_j(q')]\}, \tag{3}$$

where $W^{(ji)}_{q'q}$ is the probability of the phonon transition $\{q', j\} \to \{q, i\}$. We consider defects whose dimensions are much less than a and typical phonon wavelength which corresponds to the Rayleigh scattering regime. To obtain $W^{(ij)}_{qq'}$, it is necessary to write down the perturbation of the elastic energy caused by a defect and calculate the phonon scattering probability using the Fermi golden rule. Using the general form of the elastic energy density [2], the leading term at small q for the scattering probability can be written down as

$$W^{(ij)}_{qq'} = \frac{2\pi}{L} w_{ij} \frac{q^2 q'^2}{\omega \omega'} \delta(\omega - \omega'). \tag{4}$$

Here factors q^2, q'^2 come from the spatial derivatives of the lattice displacements in the expression for the elastic energy density, while ω and ω' in the denominator come from the expressions for the operators of the lattice displacements. In Eq. (4) L is the length of the wire; the factor 2π is introduced for simplicity. The factors w_{ij} characterize the effectiveness of the scattering and depend on the spatial distribution, concentration, and characteristics of the defects. Note that the form of Eq. (4) is provided by the defects of the elastic constants only. Contribution due to the mass defects is proportional to $\omega\omega'$. As in the case of bulk crystals, for the transitions between the 1D phonon branches having linear dispersion, the elastic-constant and mass defects provide scattering probabilities with identical dependences on the phonon wave vectors. If, however, i or j corresponds to the flexural phonons, for small q contribution of the mass defects is much less than that of the elastic-constant defects.

For the introduced form of the scattering probabilities we obtain

$$f_i^{(o)} = -\tau_i g_i \frac{\partial f_i^{(e)}}{\partial x}, \tag{5}$$

where $f_i^{(o)}$ and $f_i^{(e)}$ are odd and even parts of the distribution function and τ_i is the effective scattering time of the ith mode:

$$\frac{1}{\tau_i} = \sum_{q',j} W^{(ij)}_{qq'}. \tag{6}$$

Straightforward calculations demonstrate that if $qa \ll 1$, then the main contribution to the $1/\tau_i$ is due to the scattering where the final state belongs to one of the flexural modes, which is the direct result of their high density of states:

$$\begin{aligned}
\frac{1}{\tau_{f1}} &= \left(\frac{w_{f1f2}}{v_{f2}^{3/2}} + \frac{w_{f1f1}}{v_{f1}^{3/2}}\right) \frac{1}{qa^3 v_{f1}^{3/2}}, \\
\frac{1}{\tau_{f2}} &= \left(\frac{w_{f2f1}}{v_{f1}^{3/2}} + \frac{w_{f2f2}}{v_{f2}^{3/2}}\right) \frac{1}{qa^3 v_{f2}^{3/2}}, \\
\frac{1}{\tau_d} &= \left(\frac{w_{df1}}{v_{f1}^{3/2}} + \frac{w_{df2}}{v_{f2}^{3/2}}\right) \frac{q^{1/2}}{v_d^{3/2} a^{3/2}}, \\
\frac{1}{\tau_t} &= \left(\frac{w_{tf1}}{v_{f1}^{3/2}} + \frac{w_{tf2}}{v_{f2}^{3/2}}\right) \frac{q^{1/2}}{v_t^{3/2} a^{3/2}}.
\end{aligned} \tag{7}$$

As we see, $\tau_{f1,f2} \to 0$ as $q \to 0$. This means that semiclassical treatment of phonons by means of a kinetic equation is invalid for very small q. Introducing a characteristic frequency ω^* according to $\tau_f|_{\omega=\omega^*} = (\omega^*)^{-1}$, we restrict ourselves by consideration of regimes where $\hbar\omega^* \ll T$. In this case, the major contribution to the heat flux is provided by the well-defined phonon modes whose frequency exceeds considerably the scattering rate. Note that similar wave vector dependence of the scattering rate, as for flexural phonons, is inherent for scattering of electrons on short-range fluctuations of potential energy in the 1D case.

To determine the value of thermal conductivity we assume that $f_i^{(e)}$ have Planck form with smooth spatial variation of temperature and obtain the following expressions for the heat fluxes due to the phonons of each type, j_i:

$$
\begin{aligned}
j_{f1} &= -8\zeta(3)\,\frac{1}{\hbar^2}\,T^2 a^3 v_{f1}^{3/2}\left(\frac{w_{f1f2}}{v_{f2}^{3/2}} + \frac{w_{f1f1}}{v_{f1}^{3/2}}\right)^{-1}\frac{dT}{dx}\,,\\
j_{f2} &= -8\zeta(3)\,\frac{1}{\hbar^2}\,T^2 a^3 v_{f2}^{3/2}\left(\frac{w_{f2f1}}{v_{f1}^{3/2}} + \frac{w_{f2f2}}{v_{f2}^{3/2}}\right)^{-1}\frac{dT}{dx}\,,\\
j_{d} &= -\pi^{1/2}\zeta(3/2) v_d^3 a^{3/2}\left(\frac{T}{\hbar}\right)^{1/2}\left(\frac{w_{df1}}{v_{f1}^{3/2}} + \frac{w_{df2}}{v_{f2}^{3/2}}\right)^{-1}\frac{dT}{dx}\,,\\
j_{t} &= -\pi^{1/2}\zeta(3/2) v_t^3 a^{3/2}\left(\frac{T}{\hbar}\right)^{1/2}\left(\frac{w_{tf1}}{v_{f1}^{3/2}} + \frac{w_{tf2}}{v_{f2}^{3/2}}\right)^{-1}\frac{dT}{dx}\,,
\end{aligned}
\tag{8}
$$

where ζ stands for Riemann function. It is easy to see that at $T \ll \hbar\Delta\omega$ the dilatational and torsional phonons provide a major contribution to the heat flux and, therefore, to the thermal conductivity and thermal conductance $\sigma_T = \kappa/L$:

$$
\kappa = \pi^{1/2}\zeta(3/2)\left(\frac{T}{\hbar}\right)^{1/2} a^{3/2}\left[v_d^3\left(\frac{w_{df1}}{v_{f1}^{3/2}} + \frac{w_{df2}}{v_{f2}^{3/2}}\right)^{-1} + v_t^3\left(\frac{w_{tf1}}{v_{f1}^{3/2}} + \frac{w_{tf2}}{v_{f2}^{3/2}}\right)^{-1}\right]. \tag{9}
$$

From Eqs. (7) and (8) we can finally elucidate the role of the flexural phonons in heat transfer. First, their contribution to the heat flux is small due to their slowness and high scattering probability. Indeed, according to Eq. (4) the latter is proportional to the square of the initial phonon wave vector. If we consider phonons having energy about T, then for the flexural phonon the value of q^2 is greater than for the dilatational and torsional phonons roughly with the factor $\hbar\Delta\omega/T$. Second, as a result of their high density of states, the flexural phonons provide very effective scattering for the dilatational and torsional phonons. It is worth mentioning that the flexural phonons are important also for the nonstationary heat transfer. The latter is characterized by both thermal conductivity and thermal capacity per unit length, c. It can be easily obtained that for $T \ll \hbar\Delta\omega$ $c \sim T^{1/2}$ and the flexural phonons provide a major contribution to c, again, due to their high density of states.

An important point that is worth discussing is about the influence of the phonon localization on the heat transfer. According to the general predictions of the localization theory, if only elastic scattering is present and there is no source of dephasing, the conductance of a 1D system decays exponentially with its length L if L exceeds the mean free path of a carrier. We believe, however, that the described regime of heat transfer is not canceled by localization, in general. This is because we deal with the multichannel transfer regime where the role of distinct channels is essentially different. In particular, the main contribution to the heat flux is due to the dilatational and torsional phonons, while the flexural phonons provide a major contribution to the overall phonon density of states. Using semiquantitative arguments of Thouless [14], we expect that localization is likely to be manifested for $L > l(\hbar\Delta\omega/T)^{1/2} \gg l$, where l is the characteristic mean free path of the dilatational and torsional phonons. Nevertheless, we stress that the problem of localization definitely deserves more rigorous consideration. As we demonstrated, the peculiarities of the phonon spectrum of a wire bring about the asymptotic behavior of the phonon mean free path which is qualitatively different from that of bulk crystals. This can cause qualitatively new features of localization phenomena.

Finally, it is necessary to analyze the experimental situations where the described regime of heat transfer can be detected. This directly follows from the main assumptions we made. First, the condition $T \ll \hbar\Delta\omega$ must be satisfied. Second, phonons must be multiply scattered during the transfer through the wire. The first condition depends on the wire cross section and material parameters only, while the second one depends on the wire length and characteristics of defects. Since the characteristic phonon mean free path decreases as the temperature increases, the temperature range where the predicted heat transfer regime can be detected expands for the longer and less perfect wires. This is qualitatively illustrated in Fig. 1, where we plot schematically the temperature dependence of the wire thermal conductance. The vertical line marks the temperature where the condition $T = \hbar\Delta\omega$ is reached. The dashed line corresponds to the ballistic phonon transfer, $\sigma_T \sim T$, while the two dotted curves describe the case of intensive phonon scattering, considered in this Letter, $\sigma_T \sim T^{1/2}$. Obviously, if the wire cross section is fixed, the upper dotted curve corresponds to the wire which is either shorter or more perfect, since $\sigma_T \sim 1/(Lw)$. The two solid lines show the resulting temperature dependence of the thermal conductance. We see that in the wire that is longer or less perfect the $T^{1/2}$ law is realized in the wider temperature range and is likely to be detected. Note that some additional features, not shown in Fig. 1, can appear at temperatures below the T to $T^{1/2}$ transition. They arise because the flexural phonons are scattered much more effectively than the dilatational and torsional phonons. Therefore, at some intermediate temperatures only the dilatational and torsional phonons are ballistic. In this case $\sigma_T \sim T$, but the value of the coefficient is twice lower than for the case where all acoustic phonons are ballistic. In experiment [10] sublinear temperature dependence of the wire

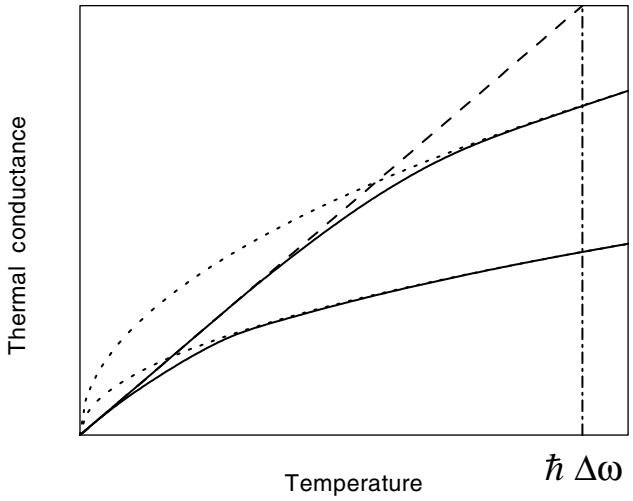

FIG. 1. Schematic temperature dependence of the wire thermal conductance in the different transport regimes. The dashed curve corresponds to the ballistic phonon transfer, the two dotted lines correspond to the phonon transfer with intensive scattering, and the solid line represents the resulting temperature dependence of σ_T. The vertical line marks the temperature where the upper phonon branches become thermally populated. The upper dotted line represents the dependence for the wire which is shorter or is characterized by less intensive phonon scattering.

thermal conductance was detected in some temperature range. However, this feature can appear not only due to the phonon scattering described in this Letter, but also due to the imperfect acoustic coupling between the wire and the reservoirs. It is necessary to undertake additional studies to determine which of these two reasons is responsible for the observed behavior.

In conclusion, we have predicted the new regime of heat transfer in nanowires at low temperatures, where only the lowest branches of the wire phonon spectrum are thermally populated. It has been demonstrated that the flexural phonons having quadratic dispersion play an especial role. They accumulate most of the wire thermal energy, practically do not contribute to the heat flux, and, finally, provide effective scattering to the dilatational and torsional phonons, which carry most of the heat flux. We have found that in this case thermal conductivity is proportional to $T^{1/2}$. Experimentally, this heat transfer regime is most likely to be detected in the samples with relatively high phonon scattering.

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