Maximizing phonon thermal conductance for ballistic membranes

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Abstract. At low temperatures, phonon scattering can become so weak that phonon transport becomes ballistic. We calculate the ballistic phonon conductance $G$ for membranes using elasticity theory, considering the transition from three to two dimensions. We discuss the temperature and thickness dependence and especially concentrate on the issue of material parameters. For all membrane thicknesses, the best conductors have, counter-intuitively, the lowest speed of sound.

1. Introduction
Recent advances in nanoscience are expanding the limits of phononic thermal transport, both in the low conductance and high conductance side [1]. The highest thermal conductance of a particular material is achieved, when the phonons do not scatter at all; this is the ballistic transport limit. At room temperature the ballistic limit is quite hard to achieve, but at low temperatures (a few K and below) phonon-phonon and phonon-impurity scattering become so weak that ballistic transport can be observed [2, 3], and the emitted power has the typical Stefan-Boltzmann form [4]

$$P = A\sigma T^4,$$

where for phonons $\sigma = \frac{\pi^5 k_B^4}{(15\hbar^3)\Sigma e_i/c_i^2}$, (1)

summing over the different phonon modes with speeds of sound $c_i$ and radiator emissivities $e_i$.

In addition to bulk samples, ballistic phonon transport was also observed for thin amorphous SiN$_x$ membranes recently [5]. At low temperatures, the dominant thermal phonon wavelength becomes comparable to the membrane thickness (for a 1µm SiN$_x$ membrane this happens at ≈100mK) leading to an effectively 2D phonon gas. To study thermal transport in nanoscale devices mounted on thin membranes, we have recently considered ballistic and diffusive thermal conduction in such membranes [6, 7, 8], spanning the transition from the 3D to the fully 2D limit, using the correct low-frequency modes known from elasticity theory. In our model, the device will uniformly heat a part of the membrane, leading to an increase of the heat flow into the rest of the membrane. Here we explicitly discuss the dependence of ballistic thermal conduction on materials parameters. The simple question we would like to answer is: what kind of material is the best (worst) ballistic thermal conductor for any thickness of the membrane, and can we even define a conductivity that only depends on the material, but not on the sample dimensions?

For the more typical cases where phonon transport is not ballistic, but limited by different scattering mechanisms in the sample, it is possible to define a material dependent local thermal...
conductivity $\kappa$, which depends on the specific heat $c_V$, average speed of sound $c$ and phonon mean free path $\Lambda$ as $\kappa = 1/3c_Vc\Lambda$. For 3D crystals, $c_V$ is proportional to $1/c^3$, but because $\Lambda$ scales as $\Lambda \propto c^n$, where $n = 3, 4, 5$ for phonon-electron, impurity, and phonon-phonon scattering, respectively, $\kappa$ always grows with higher speed of sound [4]. This is the intuitive result that high speed of sound materials are better thermal conductors (like diamond). However, for the case of ballistic conduction this is not true anymore. The thermal conductance (one cannot define a local $\kappa$ anymore) is defined as $G = \Delta P/\Delta T$. Here $\Delta P$ is the net power radiated from an object and $\Delta T$ is the temperature difference between the object and the environment. If $\Delta T$ is small, we can write $G = dP/dT$. $G$ actually has a dependence $G \propto 1/c^2$, as can be seen from the Stefan-Boltzmann law, Eq. (1). The material with the lowest speed of sound is the best thermal conductor! In the following we will investigate what is the situation for thin membranes.

2. Membrane eigenmodes

In isotropic 3D bulk systems there are three independent phonon modes, two transversally and one longitudinally polarized, with sound velocities $c_t$ and $c_l$, respectively. In the presence of boundaries, the bulk phonon modes couple to each other and form a new set of eigenmodes, which in the case of a free standing membrane are horizontal shear modes ($h$) and symmetric ($s$) and antisymmetric ($a$) Lamb modes [9]. The frequency $\omega_h$ for the $h$ modes is simply $\omega_h = c_t k^2 + (m\pi/d)^2$, where $k_\parallel$ is the wave vector component parallel to membrane surfaces, $d$ is the membrane thickness and the integer $m$ is the branch number. The dispersion relations of the $s$ and $a$ modes cannot be given in a closed form, but have to be calculated numerically [10]. The lowest three branches, dominant for thin membranes at low temperatures, have the low frequency expressions $\omega_{h,0} = c_t k_\parallel$, $\omega_{s,0} = c_s k_\parallel$ and $\omega_{a,0} = \frac{h}{2m\pi} k_\parallel^2$, with the effective sound velocity $c_s = 2c_t \sqrt{(c_t^2 - c_s^2)/c_t^2}$ of the $s$ mode and the effective mass $m^* = \hbar \left[ 2c_t d \sqrt{(c_t^2 - c_s^2)/3c_t^2} \right]^{-1}$ of the $a$ mode “particle” [10]. This lowest $a$ mode has a quadratic dispersion instead of the usual phonon-like linear one, and is mostly responsible for the non-trivial behavior of thin membranes at low temperatures.

3. Ballistic conduction

Figure 1 shows a schematic of the system in consideration. A thin metal film of perimeter $l$ heats the membrane directly below [7]. To simplify the discussion, we assume that the hot phonons from the heater have a thermal distribution and are radiated from its perimeter into the membrane, similar to black body radiation. Then we get

$$G = \frac{l}{2\pi^2} \sum_{\sigma,m \geq 0} \int dk_\parallel k_\parallel \omega_{\sigma,m} \left| \frac{\partial \omega_{\sigma,m}}{\partial k_\parallel} \right| \frac{\partial n(\omega,T)}{\partial T},$$

where $n(\omega,T)$ is the Bose-Einstein distribution and $\sigma$ and $m$ are the mode and branch indices [11]. If enough branches are used, the 3D to 2D transition can be computed from this expression. If the membrane is thin and temperature low ($Td \ll \hbar c_t/2k_B$), only the lowest branch of each mode is occupied ($m=0$), and we are fully in the 2D limit, in which case we get from Eq. (2)

$$G_{2D} = \frac{lk_B}{2\pi^2} \left[ \left( \frac{1}{c_t} + \frac{1}{c_s} \right) \Gamma(4) \zeta(3) \left( \frac{k_B T}{\hbar} \right)^2 + \frac{2m^*}{\hbar} \Gamma\left( \frac{7}{2} \right) \zeta\left( \frac{5}{2} \right) \left( \frac{k_B T}{\hbar} \right)^{3/2} \right].$$

Note that the effective mass of the lowest $a$ mode depends on the membrane thickness and hence in the 2D limit $G \propto 1/\sqrt{d}$. In the 3D limit $Td \gg \hbar c_t/2k_B$, the dominant phonon wavelength is
much smaller than \(d\), leading to decoupling of the longitudinal and transversal modes and

\[
G_{3D} = \frac{\pi^2 l d k_B}{30} \left( \frac{2}{c_t^2} + \frac{1}{c_l^2} \right) \left( \frac{k_B T}{\hbar} \right)^3 .
\]  

(4)

As expected, \(G_{3D} \propto d\). This means that at a fixed temperature \(G\) will first decrease with decreasing \(d\), then reach a global minimum and will increase again, if we decrease \(d\) further. The minimum is approximately at the 2D-3D crossover thickness \(d_C \equiv \hbar c_t/(2k_B T)\).

**Figure 1.** Schematic of the considered geometry. A thin metal film heats the part of the membrane directly below. The radiating area is \(A = l \times d\)

**Figure 2.** (a) Ballistic conductance \(G\) and (b) Ballistic conductance per unit area \(G/l d\) as function of membrane thickness \(d\). The dash-dotted line in (a) is \(\propto 1/d\).

**4. Numerical results**

Using the 300 lowest modes, we have computed the ballistic phonon conductance \(G\) for a range of parameters that spans the transition from 2D to 3D. Fig. 2 (a) shows the computed \(G\) for \(T=100\) mK and \(l=1.6\) µm as a function of the membrane thickness \(d\) for four different materials: Pb (\(c_t = 1025\) m/s, \(c_l = 2370\) m/s), Al (\(c_t = 3280\) m/s, \(c_l = 6580\) m/s), SiN (\(c_t = 6200\) m/s, \(c_l = 10300\) m/s), and poly-diamond (\(c_t = 10900\) m/s, \(c_l = 18100\) m/s). The values of \(c\) are calculated values for the isotropic case, based on measured single crystal elastic constants [12]. All materials have a physically relevant critical thickness, ranging from \(d_C = 40\) nm for Pb to \(d_C = 400\) nm in diamond, below which \(G\) increases with decreasing \(d\). The material with highest \(G\) is Pb, as it has the lowest speeds of sound, and diamond has the lowest \(G\). In the 2D limit, where \(G \propto 1/\sqrt{c}\), the differences between the materials are not as strong as in the 3D limit. One could say that all materials start to resemble each other in the ultrathin range \(d < 10\) nm.

On the other hand, in the 3D limit, \(G\) increases linearly with \(d\), the common sense result. Therefore, we could try to define a materials parameter \(G/l d\), the conductance per unit emission area, for all thicknesses. This is plotted in Fig. 2 (b). As we see, in the 3D limit \(G/l d\) is not a function of \(d\), and is truly a materials parameter. However, when the membrane becomes thinner, \(G/l d\) starts increasing strongly. This means that thin membranes are actually more effective thermal conductors, per unit emission area. This increase in ballistic “conductivity” is striking: for diamond it can be four orders of magnitude from \(d = 1\) µm to \(d = 1\) nm. Therefore,
Figure 3. Ballistic conductance $G$ as function of temperature. In the 3D limit, $G \propto T^3$, while in the 2D limit we have $G \propto T^{3/2}$.

Figure 4. Logarithmic derivative of the ballistic conductance $\alpha \equiv d \ln(G)/d \ln(T)$ as function of temperature. In the 3D limit $\alpha = 3$, while in the 2D limit $\alpha \rightarrow 3/2$.

A way of increasing the ballistic thermal conductance in a given volume would be to use a structure composed of many parallel thin membranes of a material with low speed of sound.

The dependence of $G$ on temperature is plotted in Fig. 3 for $d = 100$ nm. In the 3D limit, $G$ is proportional to $T^3$, Eq. (4). In the 2D limit however, the power of the temperature dependence does not just drop by one, but instead we have $G \propto T^{3/2}$ as it is dominated by the second term in Eq. (3), and the crossover temperature is between 50 .. 400 mK for $d = 100$ nm. To give a better picture of how the power of the temperature dependence of $G$ changes with temperature, we plot the logarithmic derivative $d \ln(G)/d \ln(T)$ of $G$ in Fig. 4.

5. Conclusions
For a given temperature, ballistic thermal conduction is maximized by choosing a material with low speed of sound, and by using several parallel thin membranes, instead of a bulk slab of the same total thickness. A bulk slab of diamond of thickness 30 $\mu$m has the same conductance as a 2 nm thick lead membrane. The lead membrane is thus about 15 000 more effective conductor. Applications in cooling ultrasensitive thermal detectors can be envisioned.

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