Heat transport in ultrathin dielectric membranes and bridges

T. Kühn, 1 D. V. Anghel, 2 J. P. Pekola, 3 M. Manninen, 1 and Y. M. Galperin 2

1 University of Jyväskylä, Department of Physics, P.O. Box 35 (YFL), FIN-40014 Jyväskylä, Finland
2 University of Oslo, Department of Physics, P.O. Box 1048 - Blindern, N-0316 Oslo, Norway
3 Low Temperature Laboratory, Helsinki University of Technology, P.O. Box 2200, FIN - 02015 HUT, Finland

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Phonon modes and their dispersion relations in ultrathin homogeneous dielectric membranes are calculated using elasticity theory. The approach differs from the previous ones by a rigorous account of the effect of the film surfaces on the modes with different polarizations. We compute the heat capacity of membranes and the heat conductivity of narrow bridges cut out of such membranes, in a temperature range where the dimensions have a strong influence on the results. In the high-temperature regime we recover the three-dimensional bulk results. However, in the low-temperature limit the heat capacity $C_V$ is proportional to $T$ (temperature), while the heat conductivity $\kappa$ of narrow bridges is proportional to $T^{3/2}$, leading to a thermal cutoff frequency $f_c = \kappa/C_V \approx T^{1/2}$.

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I. INTRODUCTION

More and more precise measurements are needed in science (e.g., in astrophysics) and therefore very sensitive detectors are required. However, even if all the technological difficulties are removed and the detector components would be perfect, the thermal fluctuations and the discreteness of particle and energy fluxes through the detector would still limit the precision of the measurements. To achieve the desired sensitivity, the detectors have to work at sub-K temperatures (to minimize the fluctuations) and have linear dimensions in the micrometer scale or even smaller (for small heat capacity and for the possibility to assemble high-resolution detector arrays for space applications). For such ranges of temperatures and dimensions, finite-size effects come into play.

Good thermal insulation of the detector is essential to attain the working temperature. For this purpose, placing the detector on top of a free-standing, amorphous and dielectric silicon-nitride (SiN$_x$) membrane appears to be a very convenient design (see, for example, Refs. 1–3). The thickness of such a membrane is of the order of hundreds of nm, which is very small as compared to its other dimensions. The membrane may also be cut, so that the detector lies on its central and wider part, which is connected to the bulk material by narrow bridges (see Fig. 1).

Thermal characteristics of SiN$_x$ membranes and bridges have been investigated experimentally by several authors (as examples, see Refs. 1 and 4–6). SiN$_x$ is an amorphous dielectric and, if we neglect here the dynamic defects (see Ref. 7 and references therein), its low temperature thermal properties are determined only by phonons. At temperatures below a few degrees K, the bulk material (assumed to be isotropic) is well described by the Debye model, with typical values for the longitudinal and transversal sound velocities $c_l = 6200$ m/s and $c_t = 10300$ m/s, respectively. Hence, the heat capacity can be expressed as $C_V = K_3 T^3$, where $T$ is the temperature and $K_3$ is a constant. If the mean free path of the phonons $l$ is assumed to vary as $l \approx \lambda^{-\nu}$, where $\lambda$ is the phonon wavelength, the heat conductivity has the expression $\kappa^{3D} = K_2 T^{3-\nu}$, where again $K_2$ is a material-dependent constant (see, for example, Ref. 9).

Note that for the above given values of sound velocity, and at temperatures below 1 K, the bulk dominant phonon wavelength $\lambda_{dom} = hc/(1.6k_B T)$ (see, Ref. 9, Chap. 8), is of several hundreds of nanometers. Thus it is comparable with the smallest dimensions of the structures measured in Refs. 1 and 4–6. Typically in these experiments, the measurements made at the lower end of the temperature interval showed qualitative differences from the measurements at the upper end of the interval, due to finite-size effects.

In this paper we will improve the model of Refs. 10 and 11 by calculating rigorously the phonon modes and their dispersion relations in ultrathin membranes and narrow bridges. We shall show the thermodynamical consequences of the calculations. Such calculations appear to be well known to those working in the field of elasticity theory (see, for example, Refs. 12 and 13), but apparently are not so familiar to the condensed matter community. Therefore, to make the paper more readable, we shall give some details of our calculations. To describe these effects, a simplified model was recently used. Namely, it was assumed that the phonon modes are quantized along the direction perpendicular to the

FIG. 1. (a) A schematic drawing of a thin free standing membrane of the type discussed in this paper. The thickness $b$ is typically a few hundreds of nm. The other dimensions $l_1$ and $l_2$ are of the order of 100 $\mu$m. (b) Such a membrane (central part) suspended to the bulk by four bridges. The bridge width $w$ ranges from few $\mu$m to tens of $\mu$m.
membrane surface. In this way, the three-dimensional (3D) (quasi-)continuous phonon spectrum splits into what one could call two-dimensional (2D) branches. \(^3\) At low enough temperatures, only the lowest branches are populated by phonons and the membrane is described as a 2D isotropic phonon gas. In this situation, if the mean free path of the phonons varies as \(l \propto \lambda^{-2}\), the heat capacity has the form \(C_V^{2D} = K_3 T^2\) and the thermal conductivity is \(\kappa^{2D} = K_4 T^{2-\gamma}\), where \(K_3\) and \(K_4\) are material-dependent constants. This model describes the change of the exponent of the temperature dependence of heat conductivity, as observed in Refs. 1, 4, and 5, and could fit relatively well the experimental data. \(^10\)

On the other hand, the observation that in narrow bridges the exponent of the temperature dependence of the heat conductivity decreases, \(^1, 3\) as well as the increase of the ratio \(\kappa/C_V\) with temperature, \(^1\) cannot be explained in this model.

II. THE MODEL

In Refs. 10 and 11 it was considered simply that the longitudinal and transversal polarized phonon modes are independently quantized by Neumann boundary conditions imposed at the membrane surfaces. Nevertheless, in a rigorous analysis it must be taken into account that the modes with different polarization couple at a free surface\(^{12}\) and because of this, the phonon modes in thin membranes are “distorted” and show features that go beyond a simple treatment of the quasi-2D phonon gas.

For concreteness, we perform calculations for the practically important case of SiN\(_4\) membranes with thickness 100–200 nm having parallel surfaces. Other dimensions of the membranes are usually of the order of 100 \(\mu m\). Consequently, the membranes can be considered as infinitely long and wide. It is further assumed that the material is isotropic. The eigenmodes of these kind of systems are well known from acoustics and are called Lamb waves.\(^{12}\)

Similar to electricity theory, the physical acoustic fields can be expressed by a scalar and a vector potential \(\Phi\) and \(\Psi\). The velocity fields of the longitudinal and transversal phonon modes are then defined as \(\vec{v}_l = \nabla \cdot \Phi\) and \(\vec{v}_t = \nabla \times \Psi\). Simple wave equations can be derived for the potentials \(\Delta \Phi = c_i^2 \partial_x^2 \Phi\) and \(\Delta \Psi = c_i^2 \partial_x^2 \Psi\). Here \(c_l\) and \(c_t (< c_l)\) are the longitudinal and transversal sound velocities, respectively. In an infinite three-dimensional space this yields one longitudinal and two transversal plane wave solutions.

When, however, the system is restricted to finite size, the boundaries of the system lead to a coupling of longitudinal and transversal modes. This coupling is due to the boundary condition at a free surface: the total stress should vanish. If the wave incident on the surface is polarized along the \(y\) direction [see Fig. 2(a)], the free boundary condition is satisfied if the reflected wave has the same polarization. Such a wave is called a horizontal shear wave (\(h\) wave). The \(h\) waves do not mix at the boundaries with waves of different polarizations and they form the typical “box eigenmodes,” with the dispersion relation

\[
\omega_{h, n, l}^2 = \left( \frac{n \pi}{b} \right)^2 + k_l^2, \quad (1)
\]

Here \(k_l\) is the component of the wave vector parallel to the membrane surface and \(b\) is the thickness of the membrane. On the other hand, if the polarization of the incident wave is either longitudinal or transversal, but in the plane \(xz\), then the reflected wave will always be a superposition of longitudinally and transversally polarized waves. These two waves have different propagation velocities, and the condition to get eigenmodes is that the plane waves reconstruct each other after two reflections. The longitudinal and transversal components of the eigenmode have the same wave vector component \(k_l\) along the membrane surfaces, but different components perpendicular to the surfaces, which we shall call \(k_t\) and \(k_t'\), respectively. The frequency of the eigenmode is then \(\omega = c_t(k_t)^2 = c_t'(k_t')^2\). These equations give a relation between the components \(k_l\) and \(k_l'\). The eigenmodes obtained in this way fall into two classes: symmetric (s wave) and antisymmetric (a wave), according to the symmetry of the velocity field of the wave with respect to the plane \(z=0\). The dispersion relation of the s and a waves are given by the equations

\[
\tan \left( \frac{b k_t}{2} \right) = -\frac{4k_t k_l k_t'}{(k_t^2 - k_t'^2)}, \quad (2)
\]

and

\[
\tan \left( \frac{b k_t'}{2} \right) = -\frac{4k_t' k_l k_l'}{(k_t'^2 - k_l^2)}, \quad (3)
\]

respectively. Equations (2) and (3), together with \(\omega = c_t^2(k_t)^2 = c_t'(k_t')^2\) form a set of transcendental equations, which can be solved only numerically. The branches of each dispersion relation are shown in Fig. 3. As can be seen, the \(h\)-modes are just usual “box modes.” Without mixing at the membrane surfaces, all the modes would be of this type and the results would be identical to the ones of Refs. 10 and 11. However, due to the coupling of the longitudinal and trans-
FIG. 3. The branches of the dispersion relations of the phonon eigenmodes of a free standing thin membrane. (a) $h$ modes, (b) $s$ modes, and (c) $a$ modes.

versal modes, the dispersion relations of the $a$ and $s$ modes show some interesting properties.

At $k_i=0$, all the excited branches satisfy the relation $\partial \omega / \partial k_0=0$, but for the $s$ and $a$ modes, unlike for the $h$ modes, $\partial^2 \omega / \partial k_i^2$ may be either positive or negative. If $\partial^2 \omega / \partial k_i^2 < 0$, the dispersion curve has a minimum at some value $k_i>0$. The lowest branch of the $h$ modes is a straight line

$$\omega_{h,0} = c_h k_i$$  \hspace{1cm} (4)

but not for the $s$ and $a$ modes. For the $s$ modes, $\partial \omega_{s,0} / \partial k_i>0$, so the group velocity of long wavelength $s$ phonons is different from zero. On the other hand, for the $a$ modes $\partial \omega_{a,0} / \partial k_i=0$ and $\partial^2 \omega_{a,0} / \partial k_i^2 > 0$. Therefore the group velocity of the $a$ modes is zero at long wavelength and from this point of view the $a$ phonons are similar to massive particles. Since the low temperature thermal properties of the membranes are determined by the dispersion relations of the low-

est branches at long wavelengths, we shall take a closer look at these.

(a) Lowest branch of the symmetric modes. If $(b/2)k_i$ converges to zero, the solutions $(b/2)k_i^l$ and $(b/2)k_i$ of Eq. (2), and satisfying $c_s^2(k_i^2) = c_i^2(k_i)^2$ approach also zero, in such a way that $k_i^l$ is real, while $k_i = ik_k^l$ is imaginary.\(^{14}\) Then Eq. (2) reduces to

$$\frac{\tan \left( \frac{b}{2} k_i^l \right)}{\tanh \left( \frac{b}{2} k_i \right)} = \frac{k_i^l}{k_i} = \frac{4 k_i^l k_i^l}{\left[ (k_i^l)^2 - k_i^l \right]^2}.$$  \hspace{1cm} (5)

The solution $k_i^l=0$ is unphysical (does not satisfy the boundary conditions if plugged into the stress formula), so the only solution is $[(k_i^l)^2 - k_i^l]^2 = 4(k_i^l)^2 k_i^l$, which yields the dispersion relation

$$\omega_{s,0} = 2 \frac{c_i}{c_i} \sqrt{c_i^2 - c_i^2 k_i} = c_s k_i.$$  \hspace{1cm} (6)

So the dispersion relation is linear in the long wavelength limit. The group velocity of the $s$ modes is $c_s$, which, since $0.5 < c_i^2/c_i^2 < 1$,\(^{14}\) takes values between $\sqrt{2} c_i$ and $2 c_i$.

(b) Lowest branch of the antisymmetric modes. In the case of antisymmetric modes, if $(b/2)k_i$ converges to zero, then both $(b/2)k_i^l$ and $(b/2)k_i$ converge to zero, but taking imaginary values: $k_i^l = ik_k^l$ and $k_i = ik_k^l$, leads to a valid solution.\(^{14}\) Expanding Eq. (3) and using the equation $\omega_s^2 = c_s^2(k_i^2) = c_i^2(k_i)^2$, we get the quadratic dispersion relation

$$\omega_{a,0} = \frac{\hbar}{2 m} k_i^2,$$  \hspace{1cm} (7)

as for massive particles of “effective mass”

$$m^* = \hbar [2 c_i b/\sqrt{(c_i^2 - c_i^2)/3 c_i^2}].$$  \hspace{1cm} (8)

A plot of the lowest branches of the $h$, $s$, and $a$-modes in the long wavelength limit is shown in Fig. 4.

III. THERMODYNAMICS

A. Heat capacity

The qualitative difference between the dispersion relations of the $a$ modes, on one hand, and the $h$ and $s$ modes, on the other hand [see Eqs. (4), (6), and (7)], have important consequences on the thermodynamic properties of the membrane. To show this, let us first calculate the heat capacity of the membrane. Phonons obey Bose statistics, so the average population of each phonon mode is $n(\omega) = 1/\exp(\beta h \omega) - 1$. If we integrate over $k_i$ and sum up the contributions of all the branches, we arrive at the expression
and $p_C$ manifest itself through a relatively rapid change of the dimensionality of the phonon gas distribution where the 3D-to-2D crossover in the phonon gas would also on $k_B T$ is the area of the membrane. The exponent of the temperature dependence of the heat capacity, following from Eq. (9), are

$$C_V = \frac{\eta_1 T^3}{k_B T^2} \sum_{\sigma} \sum_{m=0}^{\infty} \int_0^\infty dk \left( \frac{\hbar \omega_{\sigma,m}}{(\beta \hbar \omega_{\sigma,m} \exp(\beta \hbar \omega_{\sigma,m}) - 1)^2} \right),$$  

where $\sigma$ represents the $h$, $s$, and $a$ modes, while $\Sigma_m$ is the summation over the branches. The frequencies $\omega_{\sigma,m}$ depend also on $k_B$; $A$ is the area of the membrane.

For uncoupled longitudinal and transversal modes, the dispersion laws have the form $\omega = \sqrt{(\hbar n / b)^2 + \hbar^2 c^2}$. In that case the 3D-to-2D crossover in the phonon gas would manifest itself through a relatively rapid change of the temperature dependence from $T^3$ to $T^2$ at the temperature $T_c = \hbar c / 2 k_B$, as seen in Fig. 5(a). The corresponding asymptotic temperature dependences of the heat capacity, following from Eq. (9), are

$$C_V = \begin{cases} \eta_1 T^3, & T \gg T_c, \\ \eta_2 T^2, & T \ll T_c. \end{cases}$$

where

$$\eta_1 = \frac{4 \pi V k_B^4 \Gamma(5) \zeta(4)}{(2 \pi c_s h)^3} \quad \text{and} \quad \eta_2 = \frac{\pi A k_B^4 \zeta(3)}{(2 \pi c_s h)^2}.$$ 

Here, $3/c_s^3 = 2/c_1^3 + 1/c_1^3$, $3/c_s^2 = 2/c_1^2 + 1/c_1^2$, and $V$ is the volume of the membrane. The exponent of the temperature dependence of the heat capacity $p_C = \partial \ln C_V / \partial \ln T$ reflects the dimensionality of the phonon gas distribution $p_C(T \gg T_c) = 3$ and $p_C(T \ll T_c) = 2$.10,11

In the more rigorous case, i.e., when the dispersion relations are given by Eqs. (4), (6), and (7), due to the quadratic dispersion relation of the lowest $a$ mode, we get a different temperature behavior for $T \ll T_c$. Summing only over the three lowest branches, we get

$$C_V = A k_B (\alpha T^2 + \beta T),$$

where $\alpha = 3 \zeta(3) k_B^2 \frac{1 + 1/c_s^2}{\pi h^2}$ and $\beta = \frac{\zeta(3) k_B m^2}{\pi h^2}$. Preliminary estimates show that the contribution of dynamical defects to the specific heat are unimportant for such thin films; more detailed calculations are in progress. In the high-temperature limit, the expected $T^3$ behavior is obtained, but at temperatures around $T_c$, the temperature dependence of $p_C$ is somewhat more complicated, converging finally to 1, as $T \to 0$ [see Fig. 5(b)].

**B. Heat conductivity**

A common way to increase thermal insulation of the detector mounted on the membrane is to cut the membrane so
that the central part is connected to the bulk material only by narrow bridges (see Fig. 1). Therefore, another quantity of interest is the thermal conductivity ($\kappa$) along the membrane and bridges. Reported widths of the bridges of interest for us are roughly from 4 $\mu$m upwards.\textsuperscript{1,3} (We do not discuss here the “dielectric quantum wires,” as in Ref. 15.) As the width of the bridge becomes smaller than the phonon mean free path in the uncut membrane, the interaction of phonons with the bridge edges should become the main scattering mechanism. It is very difficult to solve this problem either analytically or numerically for the most general case. Instead, we shall try to extract the relevant physical results for our problem, using a realistic model. The cutting process leaves the bridge edges very rough, so we shall assume that the phonons scatter diffusively at the edges, i.e., scattered phonons are uniformly distributed over the angles and branches corresponding to the same frequency, $\omega$.

The general expression for the heat current along the rectangular bridge of total length $l$ is

$$\dot{Q} = \frac{1}{l} \sum_{\sigma,m,k} \hbar \omega(k) \tau(k) \nu^{2 \prime}_{\sigma}(k) \frac{\partial n(\omega)}{\partial T} \frac{\partial T}{\partial x},$$

where $\tau(k)$ is the (average) scattering time of a phonon having wave vector $k$, parallel to the membrane surface and belonging to the branch $(\sigma,m)$. To simplify the writing, the dependence on $\sigma$ and $m$ of the quantities in Eq. (11) was made implicit. The bridge lies along the $x$ direction, the $z$ direction is perpendicular to the membrane. We denoted the group velocity of the phonons by $v_{\sigma,m}(k) = \partial \omega_{\sigma,m}/\partial k$. We also assumed that $\partial T/\partial x$ is not too large, so that the linear approximation $\dot{Q} \approx \partial T/\partial x$ holds. Let us now denote the scattering time of the phonons in the uncut membrane by $\tau_{M,\sigma,m}(k)$, while the scattering time at the bridge edges is $\tau_{E,\sigma,m}(k)$. The effective scattering time $\tau_{E,\sigma,m}(k)$ is then

$$\tau^{-1}_{E,\sigma,m}(k) = \tau^{-1}_{M,\sigma,m}(k) + \tau^{-1}_{E,\sigma,m}(k).$$

Under the assumption of diffusive scattering at the bridge edges, $\tau_{E,\sigma,m}(k)$ can be estimated as $\tau_{E,\sigma,m}(k) = w/[v_{\sigma,m}(k) \sin \theta]$, where $\theta$ is the angle between $k_0$ and the $x$ direction, and $w$ is the bridge width. If we transform the summation over $k_0$ in Eq. (11) into an integral and write $\dot{Q} = -\kappa \partial T/\partial x$, we get

$$\kappa = \frac{w^2}{2 \pi} \sum_{\sigma,m} \int_0^{2\pi} \frac{d\theta}{w} \int_0^\infty \frac{d\omega}{v} \frac{v^2(\omega) \cos^2(\theta)}{v(\sin(\theta)) \sin(\theta)} \left( \frac{1}{\tau_M} + \frac{1}{\tau_E} \right),$$

where now $\tau_M = \tau_{M,\sigma,m}(k_0) = v_{\sigma,m}(k_0)$ is the mean free path corresponding to $\tau_{M,\sigma,m}(k_0)$. Denoting $a = w/\ell_M$ we can write the integral over $\theta$ as

$$C(a) = \int_0^{2\pi} \frac{d\theta}{\left( |\sin(\theta)| + a \right)}$$

and

$$= \frac{4}{a} \int_0^1 \frac{\sqrt{1-x^2} dx}{x + a} = \pi \frac{2}{a} - 1 + \sqrt{1-a^2} \log \left( \frac{1}{a} + \sqrt{1-a^2} \right).$$

If edge-scattering dominates, i.e., $w \ll \ell_M$, the integral only depends logarithmically on $a$.

$$C(k_0) = 4 \ln \left( \frac{2}{a} \right).$$

Considering the small bandwidth of occupied phonon modes as well as the long mean free paths in the free membranes at low temperatures, we can consider $C(a) \approx C = \text{const}$ over the temperature range that we work in.

With this effective “quasiconstant” mean free path of the phonons in the uncut membrane, we can evaluate the heat conductivity along the bridge. We did this analytically for the low-temperature limit of a quasi-2D phonon gas and numerically for higher temperatures. The analytical low-temperature limit gives

$$\kappa = \frac{C \hbar^2 k_B}{2 \pi} \left[ 6 \xi(3) \left( \frac{1}{c_i} + \frac{1}{c_s} \right) \left( \frac{k_B T}{h} \right)^2 + \sqrt{\frac{2m^*}{8 \pi} \frac{3}{2} \epsilon(5/2)} \right] \times \left( \frac{k_B T}{h} \right)^{3/2},$$

so in the limit of low temperatures $\kappa \propto T^{3/2}$. The numerical results are shown in Fig. 5(c).

If a membrane, which is connected to the bulk material by narrow bridges, is heated by an ac current, its thermal cutoff frequency has the expression $f_c = G/C \approx 1/|C_V|$, where $\kappa$ is the thermal conductivity of the bridge and $C_V$ is the heat capacity of the membrane. If all the modes are of the form (1) (uncoupling of the phonon polarizations at the membrane surfaces), then both, $C_V$ and $\kappa$, are proportional to $T^5$ in the limit of low temperatures (see Refs. 10 and 11) and $f_c = \text{const}$. On the other hand, using Eqs. (10) and (13) we obtain $f_c \propto T^{12}$ in the low-temperature limit. The numerical results are plotted in Fig. 6. The increase of $f_c$ with $T$ was observed experimentally in Ref. 1, but for a wider temperature range.

IV. CONCLUSIONS

In summary, we used elasticity theory to calculate the phonon modes in ultrathin membranes made of homogeneous, isotropic silicon nitride (SiN). Using the dispersion relations thus obtained, we calculated the heat capacity and heat conductivity of the membrane and of bridges, cut out of such membranes. In the low-temperature limit the phonon gas becomes two-dimensional and populates three branches of the dispersion relations, namely the lowest $h$, $s$, and $a$ branches (see Fig. 3). At low temperatures, the dispersion relation corresponding to the lowest $a$ branch is quadratic in $k$, while the other two are linear, so at low temperatures the
a branch gives the dominant contribution. Quite surprisingly, this implies that the universal behavior of heat capacity in two-dimensional systems is obeyed also by the phonon gas at low temperatures, where $C_V \sim T$ (see Ref. 16, and references therein).

In the calculation of thermal conductivity along bridges, we assumed diffusive scattering of phonons at the bridge edges. This is justified by the fact that the cutting process leaves these edges very rough. If the width of the bridge decreases below a certain value (depending on the mean free path of the phonons in the uncut membrane) the interaction with the edges becomes the main scattering process for the phonons, see Eq. (12). In such a case, at low temperatures it was found that $\kappa \sim T^{3/2}$ [Eq. (13)].

If a membrane, connected to the bulk material by narrow bridges, is heated by an ac current, the amplitude of the temperature oscillations in the membrane has a cutoff around the frequency $f_c = G/C_V$. In the low-temperature limit, this cutoff frequency shows an increase with the temperature, as $T^{1/2}$. Preliminary experimenatal results show an increase of $f_c$ with $T$, but on a temperature range much wider than the one in Fig. 6. This seems to suggest that at higher temperatures other processes have to be taken into account in the calculation of thermal characteristics of SiNx membranes.

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