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Size dependent thermal conductivity of Si nanosystems based on phonon gas dynamics

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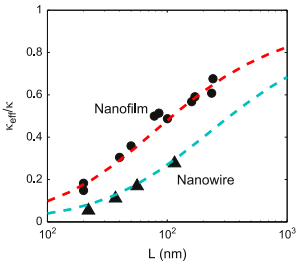
HIGHLIGHTS

- We establish a phonon gas model for thermal conduction in nanosystems.
- We obtain a linear size dependent phonon gas viscosity in Si nanosystems.
- We obtain an explicit expression for thermal conductivity of Si nanosystems.

GRAPHICAL ABSTRACT



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ABSTRACT

The silicon nanosystems have shown a great potential for high efficient energy conversion devices due to the strong size effect on thermal conductivity. An accurate and convenient prediction model for such size effect is highly desired. In this paper a macroscopic heat conduction model for nano-systems is presented based on the phonon gas dynamics, in which heat conduction is regarded as phonon gas flow in a porous medium. The resistant term in the momentum equation of the phonon gas flow consists of two parts. One is the Darcy's term, representing the volume resistance and another is the Brinkman term, representing the surface resistance. The latter is usually negligible compared with the former for the medium at the normal scale, while the relative importance of the Brinkman term increases and consequently, the thermal conductivity decreases with size reduction. The effective phonon gas viscosity is extracted from the experiments and found to be proportional to the system size in nanoscale based on the rarefied gas dynamics. In this way an explicit expression for the size dependent thermal conductivity of silicon nanosystems is obtained, which agrees well with the experimental results for both nano-wires and films.

1. Introduction

The effective thermal conductivity (κ_{eff}) of nanosystems is shown to depend on their characteristic sizes [1–21]. The κ_{eff} can be much decreased in nanosystems, such as nanofilms and nanowires of semiconductors. The size effect of κ_{eff} reveals a great potential of nano-engineered devices in the field of high efficient energy transport and conversion, which stimulates much research in the past decade. In particular, the doped and etched rough boundary silicon nanowires have been observed to have a high figure of merit (ZT) [2–3]. Such merit is mainly attributed to the extremely low thermal conductivity of the nanowires in experiments (1–10% percent of the bulk value). A large number of theories have been developed to explain the experimental observations and model the size dependent behavior of κ_{eff} in nanoscale. The Boltzmann transport equation (BTE) [9–10], molecular dynamics simulation (MD) [9–17], and Monte Carlo simulation (MC) [17–21] have obtained similar results to the experiments.

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Models with minimal fitting parameters and simple calculation are also proposed to fast evaluate the thermal conductivity of nanosystems [22–32], without integral details over frequency spaces or atomistic calculations. These methods are reasonable for nanosystems thicker than 20 nm, where the phonon density function has no significant difference from the bulk materials [9]. The gray model [22–23] estimates the nanoscale thermal conductivity with the mode-independent phonon velocity and relaxation time, and uses the Matthiessen rule for mean free paths (MFPs) reduced by the diffuse boundary scattering. Alvarez and Jou [24] derive an explicit expression of the thermal conductivity of nanofilms depending on the Knudsen number, by assuming the characteristic heat wave length equals the nanofilm thickness. McGaughey et al. [25] propose a new model with the Debye approximation for the phonon dispersion, the Matthiessen rule for MFPs, as well as the directional dependent group velocity and relaxation time. A similar assumption was also used to investigate the thermal conductivities of core-shell nanostructures by Lü [26].

There are different views on the magnitude of effective phonon MFPs in these models. Based on the traditional Debye model, the effective phonon MFP of Si at room temperature is around 40–43 nm, which is used in Alvarez and Jou's model [24]. Gang and Yang [33,34] proposed that the optical phonon contributes little to the thermal conduction, while the average phonon group velocity should be modified according to the dispersion relation. Therefore, the MFP of Si is around 260 nm, with which the gray model approximately agrees with the nanofilm experiments. Yang and co-workers [15] estimated that the MFP of Si is about 60 nm based on the phonon relaxation time calculation. Dames and Chen [35] obtained the MFP of Si as 210 nm based on a sine-dispersion approximation, which is recently adopted by Ma [32] in his phonon hydrodynamic model. However, while most of the above models predict well the κ_{eff} of nanofilms compared with experiments, they generally overestimate the κ_{eff} of nanowires.

The phonon hydrodynamics (PH) model [27–32] based on the solution of the phonon Boltzmann transport equation accounts for the boundary scattering through a continuum mechanics viewpoint. The PH model has a Laplacian term of the heat flux, $\nabla^2 q$, like the viscous stress term in fluid mechanics. Therefore, the phonon gas is supposed to form a Poiseuille flow in nanosystems when the MFPs are much larger than the system size. The boundary drag is transmitted from the boundary to the inside through the phonon gas viscosity. Solutions with different boundary conditions, such as the Maxwell boundary [29,30], backscattering boundary [31] and MFP-proportional slip boundary [32], have been proposed and model the size dependent κ_{eff}. However, the comparison of PH models with experiments at present is mainly qualitative. Similar macroscopic model is presented by the thermomass model [36–43], which regards the phonon gas as a real weighable fluid and establishes a general heat conduction model by means of gas dynamics. The thermomass model elucidates that phonon gas flow in the normal scale media is like the Darcy flow in porous media, while the boundary effects are negligible. When the system size shrinks to nanoscale, the Laplacian term of heat flux appears in the transport equation as a Brinkman extension, leading to a similar heat conduction equation to the PH model. This paper aims to investigate the nanoscale heat conduction from the viewpoint of phonon gas dynamics. Analysis of rarefied phonon gas dynamics leads to a simple quantitative expression for predicting the size dependent κ_{eff}.

2. The Poiseuille flow model based on phonon hydrodynamics

The idea that phonons act like gases can be traced back to 1920 s, proposed by Debye et al. They predicted the thermal conductivity in terms of MFP, just like in kinetic theory of gases [44–45]

$$\kappa = \frac{1}{3}\rho C_V v_s l_R \tag{1}$$

where κ is the thermal conductivity, ρ is the density, C_V is the specific heat at constant volume, v_s is the phonon group speed, and l_R is the MFP, i.e. average distance traveled by phonons between momentum non-conserving collisions, such as Umklapp scattering or defects scattering. For room temperature Si, the usually adopted value of l_R is 42 nm with the properties as shown in Table 1.

Table 1
Properties used for bulk Si at 300 K.

κ	ρ	C_V	v_s	γ_G
148 W/(m K)	2330 kg/m^3	707 J/(kg K)	6400 (m/s)	1.96

Guyer and Krumhansl [27–28] solved the phonon Boltzmann equation by a linear assumption and obtained a transport model (GK model) containing the transient and nonlocal terms

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{1}{3}v_s^2 \nabla E = -\frac{\mathbf{q}}{\tau_R} + \frac{\tau_N v_s^2}{5}(\nabla^2 + \zeta \nabla\nabla)\mathbf{q} \tag{2}$$

where $\boldsymbol{q}$ is the heat flux, v_s is the average speed of phonons, $\boldsymbol{E}$ is the internal energy density, τ_R and τ_N are the relaxation time for resistive scattering (R process) and normal scattering (N process), respectively. ζ is a numerical factor, whose value is 2 [27] or 1/3 [47], due to different integral ways. The GK model is similar to the Navier–Stokes (NS) equation because of the second order derivative term of heat flux. In particular, the quantity $\boldsymbol{u}=3\boldsymbol{q}/\rho C_V T$ is called the fluid velocity of phonon gas. For steady heat conduction in straight wires or films, the GK model can be simplified as

$$\kappa \nabla T = -\mathbf{q} + \frac{l_R l_N}{5}\nabla^2 \mathbf{q} \tag{3}$$

where $l_R = v_s \tau_R$ and $l_N = v_s \tau_N$ are the MFPs of the resistive scattering and normal scattering, respectively. The thermal conductivity κ is the same as in Eq. (1). The nonlocal term, $\nabla^2\boldsymbol{q}$, suggests that the heat flux in a wire or film is non-uniform in each cross section. If $\nabla^2\boldsymbol{q}$ is negligible, Eq. (3) reduces to the normal Fourier's law. If $\nabla^2\boldsymbol{q}$ dominates, Eq. (3) has a form like NS equation and predicts a parabolic heat flux profile like the Poiseuille flow. The question is in which condition the nonlocal term should be taken into account. A characteristic length can be defined as

$$l_G = \sqrt{\frac{l_R l_N}{5}} \tag{4}$$

and its ratio over the characteristic size of the nanosystem is measured by a Knudsen number, $\mathrm{Kn}_G = l_G/L$, where L is the thickness of films or the diameter of wires. Note that the characteristic length l_G is different from the ordinary mentioned MFP. The latter is l_R in general. The Poiseuille flow of phonon gas forms when the $\mathrm{Kn}_G \gg 1$, i.e. the term, $l_G^2\nabla^2\boldsymbol{q}$, overwhelms $\boldsymbol{q}$ in Eq. (3). At this time the phonon gas is governed by

$$\kappa \nabla T = l_G^2 \nabla^2 \mathbf{q} \tag{5}$$

Assume a non-slip boundary condition, the effective thermal conductivity, κ_{eff}, can be easily obtained as [29–30]

$$\kappa_{eff} = \frac{1}{A}\kappa \mathrm{Kn}_G{}^{-2} \tag{6}$$

where A is the numerical parameter depending on the cross section shape, $A=12$ for films, $A=32$ for wires. Eq. (6) implies that κ_{eff} is proportional to L^2, which deviates from the experimental results. To mend this, Jou et al. proposed a Maxwell slip boundary condition instead of the non-slip boundary condition [29–30] for nanosystems with strong size effects. It is assumed that the slip velocity (heat flux) on the walls is proportional to the MFP times the velocity gradient on the surface,

$$\mathbf{q}_{\mathrm{w}} = -Cl_R \frac{\partial q}{\partial r}|_w \tag{7}$$

where C is the slip parameter related to the properties of the walls. Therefore, if $\mathrm{Kn}_G \gg 1$, the κ_{eff} shows a linear dependence on the system size,

$$\kappa_{eff} \propto \kappa \mathrm{Kn}_G{}^{-1} = \kappa L/l_G \tag{8}$$

which qualitatively agrees with experiments.

It is concluded from Eq. (3) that the reduction due to boundary drag is worth considering only when l_G is comparable with or larger than the system size, L. To ensure the validity of Eq. (3), which is a macroscopic continuum equation like the NS equation, the momentum exchange by normal collision should be more frequent than that by the resistive one. Therefore, there exists a window for the Poiseuille flow of phonon gas [28],

$$l_N \ll L, \quad l_G \gg L \tag{9}$$

This condition is hardly satisfied according the temperature dependent feature of MFPs. Moreover, there are few reference values for l_N, limiting the applicability of Eq. (3) to predict the κ_{eff} in real experiments. The experiment in Poiseuille flow region should be a good way to measure l_N, however, no convincing result has been achieved. In previous discussion on nanosystem heat conduction, the role of l_N has not received much attention. Models based on the GK model usually adopt l_R instead of l_G in Eq. (3).

3. The Darcy–Brinkman model based on the phonon gas dynamics

The thermomass theory [36–43] treats the phonon gas as a weighable fluid based on the mass energy equivalence. The mass density of phonon gas is $\rho_{\mathrm{h}}=\rho C_V T/c^2$, with c the vacuum light speed. The drift velocity of phonon gas is defined as $\boldsymbol{u}_{\mathrm{h}}=\boldsymbol{q}/\rho C_V T$, which is similar to the definition of "fluid velocity" in Ref. [27]. The transport equation of the phonon gas is established as a fluid flow in the porous media

$$\rho_h \frac{\partial \mathbf{u}_{\mathrm{h}}}{\partial t} + (\rho_h \mathbf{u}_{\mathrm{h}} \nabla)\mathbf{u}_h + \nabla p_h = \mathbf{f}_h \tag{10}$$

where p_h is the phonon gas pressure

$$p_h = \gamma_G \rho_h C_V T = \frac{\gamma_G \rho (C_V T)^2}{c^2} \tag{11}$$

with γ_G the Grüneisen parameter. The first and second terms on the left hand side of Eq. (10) is the inertia (acceleration) terms, the third term is the driving term and $\boldsymbol{f}_h$ is the friction term. The previous version of thermomass theory assumed that $\boldsymbol{f}_h$ is proportional to the drift velocity of phonon gas and in a reverse direction, which is the same as the Darcy's law, i.e. $\boldsymbol{f}_h \propto -\boldsymbol{u}_h$. This assumption permits Eq. (10) to reduce to the Fourier's law when the inertia terms are negligible. In this sense, the heat conduction is similar to the porous flow, and the Fourier's law corresponds to the Darcy's law.

However, the Darcy's law is only a coarse description for the porous flow in large scale material. For a general constitutive equation of porous flow, the effects of acceleration, nonlinear drag and advection should be included [48–51]. The Brinkman's equation is a well-known generalization to the Darcy's law,

$$\mathbf{f} = -\frac{\mu}{K}\mathbf{u}_m + \mu \nabla^2 \mathbf{u}_m \tag{12}$$

where $\boldsymbol{f}$ is the total resistance, $\boldsymbol{u}_{\mathrm{m}}$ is the velocity of fluids, μ is the viscosity of the fluid, and K is the permeability. The first term in Eq. (12) leads to the Darcy flow, so we call it the Darcy friction term. The second term in Eq. (12) is introduced from the normal fluid flow, and is called the Brinkman term. The Brinkman term describes the advection effect. The characteristic length, $l_B=K^{1/2}$, reflects the attenuation length of boundary effect [51]. Therefore, the dimensionless Brinkman number, $\mathrm{Br}=l_B/L$, weighs the importance of viscous friction compared with the Darcy friction. If $\mathrm{Br}\ll 1$, the boundary effect region is much smaller that the channel width, then the velocity profile is nearly uniform at the cross section, which agrees with the prediction of Darcy's law. Conversely, if $\mathrm{Br}\gg 1$, the flow is mainly impeded by the boundary drag, thus the velocity profile approaches to the Poiseuille flow.

In analogy with Eq. (12), the friction term in Eq. (9) is rewritten as

$$\mathbf{f}_h = -\beta \rho_h \mathbf{u}_h + \mu_h \nabla^2 \mathbf{u}_h \tag{13}$$

where β is the friction parameter, μ_h is the viscosity of phonon gas. The characteristic length turns to

$$l_B = \sqrt{\mu_h/\beta\rho_h} \tag{14}$$

When the system size is large, the Brinkman term in Eq. (13) is negligible. The inertia term is also negligible if we consider the steady flow in straight systems. In this condition Eq. (10) reduces to the Fourier's law and the relation between the thermal conductivity and the friction factor yields,

$$\beta = 2\gamma_G \rho C_V^2 T/\kappa \tag{15}$$

The previous work [36–43] indicates that the relaxation time for R process is

$$\tau_R = \frac{\kappa}{2\gamma_G \rho C_V^2 T} \tag{16}$$

Therefore, Eq. (15) can be further simplified as $\beta = 1/\tau_R$. For steady conduction in straight nanosystems, we obtain the constitutive equation for heat conduction in small systems by inserting Eqs. (13–16) into Eq. (10) and dropping the inertia terms,

$$-\kappa \nabla T = \mathbf{q} - \frac{\mu_h \tau_R}{\rho_h}\nabla^2 \mathbf{q} = \mathbf{q} - l_B^2 \nabla^2 \mathbf{q} \tag{17}$$

It is obvious that if we set $l_B=l_G$, Eq. (17) is the same as Eq. (3). The difference between them is that Eq. (3) is derived from the linear Boltzmann equation while Eq. (17) is from the governing equation of phonon gas flow in porous media. Therefore, they can be regarded as the microscopic and macroscopic interpretation of the same governing equation, respectively. Analysis based on the phonon Boltzmann derivation also shows that the Brinkman term rises microscopically from the Chapman–Enskog expansion to the distribution function [39], which is exactly the same as microscopic foundation of the viscous stress term in NS equation. Similarly, recent work [46] also indicates that a hydrodynamic description is possible for localized electromagnetic waves in complex open systems.

The analytical solution to Eq. (17) describing the Darcy–Brinkman (DB) flow of phonon gas is obtained by previous work [28–31]. The geometries considered are nanofilms (NFs) and nanowires (NWs), as shown in Fig. 1. The heat flow is in the x direction. If l_B is constant, and the heat flux vanishes on

boundaries, the heat flux profile in a NF is

$$q(r) = -\kappa \nabla T \left[1 - \frac{\cosh(r/l_B)}{\cosh(L/2l_B)}\right] \tag{18}$$

where $r \in [0, L/2]$ is the distance from the central line. This solution agrees with the model in Ref. [52] which indicated an attenuation of ballistic distribution function from the boundary. Then κ_{eff} is defined by the integral

$$\kappa_{eff}^{nf} = \frac{\int_L q\, dy}{-\nabla T L} = \kappa_0 \left[1 - 2\mathrm{Br}\, \tanh(1/2\mathrm{Br})\right] \tag{19}$$

For NW the heat flux profile is

$$q(r) = -\kappa \nabla T \left[1 - \frac{J_0(ir/l_B)}{J_0(iR/l_B)}\right] \tag{20}$$

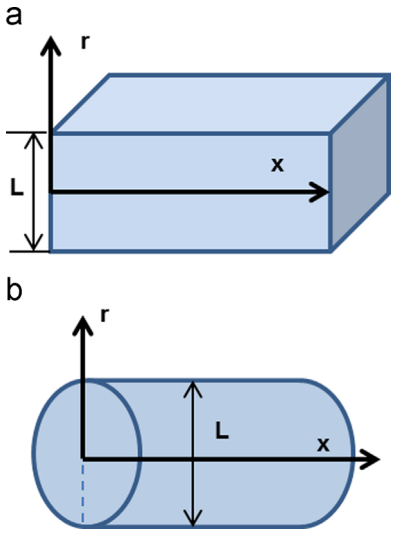

Fig. 1. Geometry of (a) Nanofilm and (b) Nanowire.

where R is the radium of wire and J is the cylinder Bessel function as

$$J_n(x) = \left(\frac{x}{2}\right)^n \sum_{t=0}^{\infty} \frac{(-1)^t (x/2)^{2t}}{t!(t+n)!} \tag{21}$$

Thus the κ_{eff} is

$$\kappa_{eff}^{nw} = \kappa \left[1 - (4\mathrm{Br}) \frac{J_1(i/2\mathrm{Br})}{iJ_0(i/2\mathrm{Br})}\right] = \kappa \left[1 - \frac{\sum_{t=0}^{\infty} \frac{(4\mathrm{Br})^{-2t}}{t!(t+1)!}}{\sum_{t=0}^{\infty} \frac{(4\mathrm{Br})^{-2t}}{t!t!}}\right] \tag{22}$$

In Fig. 2 the illustrative solutions of the NS model, Eq. (5), and DB model, Eq. (17), are presented for NFs. For comparison we assume $l_G = l_B$, thus $\mathrm{Kn}_G = \mathrm{Br}$. At small Br the NS model predicts a huge flow rate, with the maximum q much larger than q_0. For the DB model, the viscous layer is constrained in the near boundary region, with the central flow region having a uniform heat flux q_0. As Br grows, the profile of the NS model is asymptotic to the DB model. The difference of the predicted κ_{eff} between the NS model and DB model is 9.1% at Br = 1, and 0.6% at Br = 4. It implies that neglecting the Darcy friction term could cause considerable error at intermediate size.

4. Rarefied phonon gas dynamics and κ_{eff} of nanosystems

In the porous flow of ordinary fluid, l_B is generally much larger than the MFP of fluid. So the magnitude of Br does not affect the applicability of the macroscopic continuum equation. The solution of Eq. (12) with a constant viscosity is accurate enough. However, for phonon gas flow in nanosystems, l_B is probably in the same magnitude of l_R and l_N. Therefore, the rarefaction effect should be simultaneously considered for the latter.

The behavior of gas flow at high Knudsen number has received much investigation [53–59]. Microscopic methods including solving the Boltzmann equation [53,54] and direct simulation

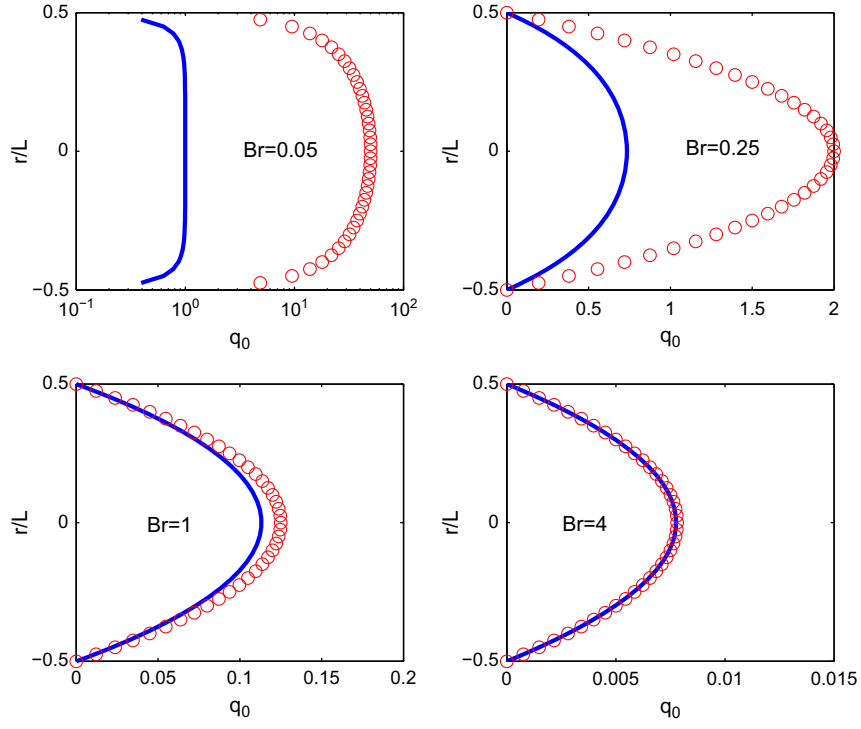

Fig. 2. The velocity profile based on NS model (Circles) and DB model (Lines) at different Brinkman numbers (Br). Here κ is the thermal conductivity of bulk sized Si, $q_0 = -\kappa \nabla T$ is the unit heat flux in bulk material.

Monte Carlo [55,56] agree with the experimental observation [57] that the effective viscosity of fluid will reduce from the bulk at high Kn, as well as the non-slip boundary yields to the slip boundary. Macroscopic continuum models have also been proposed to facilitate the multi-scale numerical work, which is able to capture the main feature of the flow while avoid much calculation cost. Such model should include the effects of effective viscosity reduction (EVR) or boundary velocity slip (BVS). The EVR effect refers to the velocity profile deviation from that based on the constant viscosity, while the BVS effect refers to the non-zero velocity at boundary. Both effects predict an increase of volume flow rate compared with the nonslip Poiseuille flow. It is not clear which one is more convenient to use in the rarefied phonon gas model, as well as which one is more responsible in physical sense. Sellitto et al. [30,31] showed that using a slip boundary with a constant slip parameter, C, the quadratic dependence of κ_{eff} is reduced to a linear dependence on size. Nevertheless, they didn't discuss the possibility to use an EVR model. Therefore, here we would like to investigate the rarefaction effect of phonon gas flow from an EVR viewpoint.

There are some models for the EVR effect in rarefied gas dynamics. Based on the solution to the linearized Boltzmann equation for the Couette flow problem, Veijola and Turowski [58] proposed an expression for the effective viscosity, μ_{eff}, as

$$\frac{\mu_{eff}(\mathrm{Kn})}{\mu} = \frac{1}{1+2Kn+0.2\mathrm{Kn}^{0.788}\exp(-\mathrm{Kn}/10)} \tag{23}$$

where μ is the viscosity in bulk limit, λ is the MFP of gas, $\mathrm{Kn}=\lambda/L$ is the Knudsen number. Here the viscosity is evaluated by the ratio of shear stress over velocity gradient, as

$$\mu_{eff} = -\frac{\langle \tau_{xy}\rangle}{\langle \partial u/\partial y\rangle} \tag{24}$$

where the angle bracket means average. Another model is proposed by Guo et al. [59] based on the MFP suppression calculation. For a 2D channel, the local effective viscosity is given as

$$\frac{\mu_{eff}(r)}{\mu} = 1+\frac{1}{2}\left[(\alpha-1)e^{-\alpha}+(\beta-1)e^{-\beta}-\alpha^2E_i(\alpha)-\beta^2E_i(\beta)\right] \tag{25}$$

where

$$\alpha=\frac{L/2-r}{\lambda},\quad \beta=\frac{L/2+r}{\lambda},\quad E_i(x)=\int_1^\infty t^{-1}e^{-tx}\,\mathrm{d}t \tag{26}$$

The spatial dependent viscosity is then incorporated with the normal constitutive relation to form the extended Navier–Stokes constitution (ENSC). The ENSC is reported to be able to characterize the velocity profile of rarefied gas flow, which implies that the viscosity decrease actually happens in the Knudsen layer. Based on ENSC, we obtain the flow rate, Q, under unit pressure drop. Therefore, the average effective viscosity is evaluated through the flow rate

$$\mu_{eff}(\mathrm{Kn}) = -\frac{1}{12}\frac{L^3W}{Q(\mathrm{Kn})}\frac{\partial p}{\partial x} \tag{27}$$

where W is the unit width. In Fig. 3 the Kn dependence of μ_{eff} based on Veijola's model and Guo's model are plotted. Both models predicts that when $\mathrm{Kn}\gg 1$, μ_{eff} is approximately proportional to Kn^{-1}, in other words, proportional to the characteristic size of systems. At large Kn the μ_{eff} based on Guo's model is twice as that on Veijola's model. The discrepancy is possibly due to the different viewpoint of evaluating μ_{eff} in each model, i.e. Eqs. (24) and (27).

In both Veijola and Guo's models, the EVR is not meant to exclude the existence of BVS. Instead, it can be regarded as an alternative simplified model which inclusively describes rarefaction effects. Thus it is reasonable to use EVR to characterize the rarefied phonon gas flow. The effective l_B is extracted from

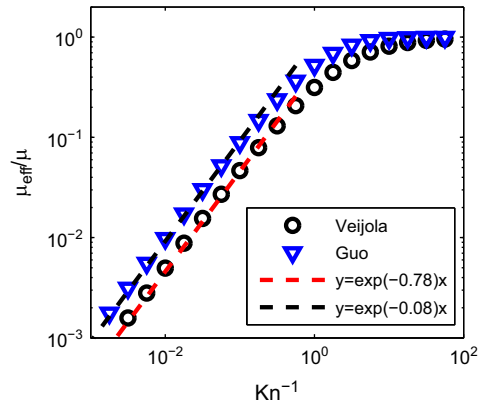

Fig. 3. The effective gas viscosity (μ_{eff}) vs. Knudsen number (Kn) based on Veijola's model (Eq.(23)) and Guo's model (Eq. (25)). μ is the gas viscosity in normal size systems.

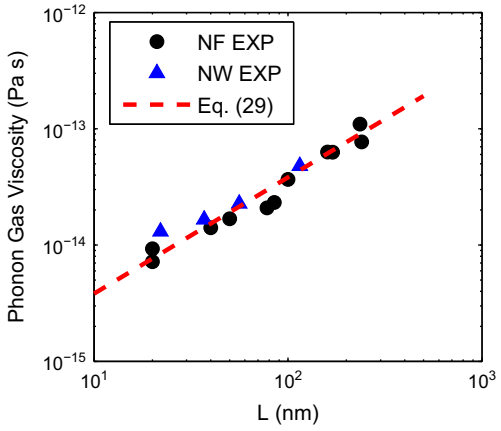

Fig. 4. The effective viscoisty of phonon gas ($\mu_{(h)eff}$) of Si nanosystems based on experiments. Experiment data is from [5–8].

Eqs. (19) and (22) with the experimental data [5–8] which present κ_{eff}/κ at each system size. Then the effective phonon gas viscosity $\mu_{(h)eff}$ is expressed as

$$\mu_{(h)eff} = \frac{2\gamma_G\rho^2C_V^3T^2}{c^2}\frac{l_B^2}{\kappa} \tag{28}$$

The properties for Si at 300 K are listed in Table 1. The obtained $\mu_{(h)eff}$ is plotted against system size in Fig. 4. It is shown that for these nanosystems, the $\mu_{(h)eff}$ can be well approximated by a linear relation

$$\mu_{(h)eff} = \varepsilon L \tag{29}$$

where the linear factor $\varepsilon = 3.83\times10^{-7}$ Pa s m^{-1}. Inserting Eq. (29) into Eq. (14) the effective l_B in each size yields

$$l_B = \sqrt{\frac{\kappa c^2\varepsilon L}{2\gamma_G\rho^2C_V^3T^2}} = \sqrt{\lambda_E L} \tag{30}$$

where $\lambda_E = 7.53$ nm is a coefficient with a unit of length. From the above analysis we see that λ_E should depend on the material properties and temperature. It is a constant for the present system due to the linear dependence of $\mu_{(h)eff}$ on L.

The strong linear dependence on size is in analogy with that predicted by rarefied gas dynamics such as Veijola's model and Guo's model. It indicates that the EVR is a convenient way to model the phonon gas flow in nanosystems.

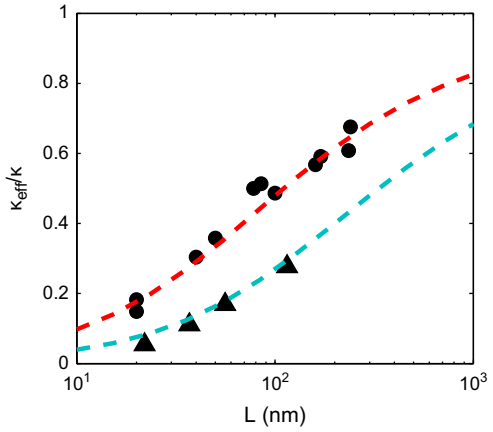

Fig. 5. The effective thermal conductivity (κ_{eff}) of Si nanosystems predicted by the phonon gas model compared with the experimental data. κ is the thermal conductivity of bulk sized Si. Circle dots: experimental data for nanofilms [5–7]; Triangle: experimental data for nanowires [8]; Upper Dash Line: Eq. (31a); Lower dash line: Eq. (31b).

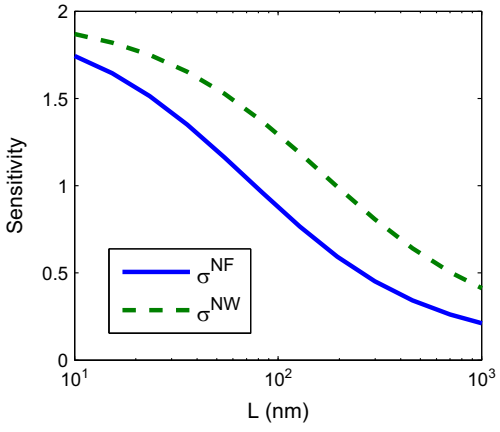

Fig. 6. Sensitivity of our model for nanofilms (σ^{NF}) and nanowires (σ^{NW}) at different system sizes. σ refers to the variation of κ_{eff} induced by the unit fluctuation of l_B and is given by Eq. (33).

Inserting Eq. (30) into Eqs. (19) and (22), we obtain the explicit expression for the κ_{eff} of Si nanosystems at 300 K, i.e.

$$\kappa_{eff}^{nf} = \kappa\left[1-2\sqrt{\frac{\lambda_E}{L}}\tanh\left(\frac{1}{2}\sqrt{\frac{L}{\lambda_E}}\right)\right] \tag{31a}$$

$$\kappa_{eff}^{nw} = \kappa\left[1-\frac{\sum_{t=0}^{\infty}\frac{(L/16\lambda_E)^t}{t!(t+1)!}}{\sum_{t=0}^{\infty}\frac{(L/16\lambda_E)^t}{t!t!}}\right] \tag{31b}$$

The predicted results are compared with experiments in Fig. 5. It can be seen that the present model predicts well the κ_{eff} of both nanofilms and nanowires.

The contribution to the temperature drop from the Darcy friction is

$$\varphi_D = \frac{\int_L q\,dy}{-\kappa\nabla T L} = \frac{\kappa_{eff}}{\kappa} \tag{32}$$

Thus κ_{eff}/κ represents the percentage occupied by Darcy friction in the total friction at different system sizes. In nanosystems it evidently reduces from unity because the importance of Brinkman friction increases. However, Fig. 5 shows that even in 20 nm systems the Darcy friction contributes over 10% to the total temperature drop, while in 100 nm systems the contribution is near 50%. It infers that the DB flow model is more suitable than the NS equation for the phonon gas flow in nanosystems, especially for those with an intermediate thickness of around 100 nm.

Since the present l_B is extracted from the experimental results, we want to know the error in this algorithm. The sensitivity is defined as

$$\sigma = \left|\frac{\partial\kappa_{eff}/\kappa_{eff}}{\partial l_B/l_B}\right| \tag{33}$$

The analytical expression for the sensitivity can be derived from Eqs. (19) and (22). Here we just present the numerical results for the sensitivity of l_B, as shown in Fig. 6. The σ is high for small systems, since the Brinkman term is significant. For large systems, the Darcy term is the main contributor to κ_{eff}, so the variation of l_B has less impact on κ_{eff}. The σ decreases by an order of magnitude when L varies from 10 nm to 1 μm. Therefore, the uncertainty is larger for the calculated l_B for larger systems. Also, the σ is larger for nanowires than for nanofilms, because the nanowires have stronger suppression on the MFPs, and thereby the Brinkman term occupies a larger fraction. It means that the estimation based on nanowire experiments can be more accurate.

5. Concluding remarks

The previous theories on the size dependent κ_{eff} are mostly based on the MFP suppression, which is a microscopic view on the mechanism of the size effect. Although these models obtain similar results to experimental data, there is some controversy about the value of MFP, and its dependence on geometry is unclear. The phonon hydrodynamics model based on the solution of Boltzmann equation characterizes the heat conduction in high *Kn* limit by the Navier–Stokes equation combined with a slip boundary condition, leading to a linear size dependent behavior of κ_{eff}. The size and geometry dependence is thereby attributed to the boundary induced viscous effect. However, the size dependent thermal conductivity predicted by the PH model is compared with the experimental data only for Si nanowires at low temperature, and the large fluctuation of slip parameters makes the model inconvenient to use.

In the present work, we macroscopically derive the constitutive equation for a phonon gas flow in a porous flow based on phonon gas dynamics. The phonon gas, unlike the phonon hydrodynamics model, is impeded by two effects: the first is the bulk friction proportional to its drift velocity, which is the Darcy term; the second is the viscous friction coming from the boundary, which is the Brinkman term. The Brinkman term with respect to the Darcy term is significant only for nanosystems, and the boundary effect is attenuated with a characteristic length, l_B. For different geometries, the boundary resistance can be explicitly weighed by the solution of the Darcy–Brinkman flow model.

To model the κ_{eff} of nanosystems, a size dependent effective viscosity is inserted into our Darcy–Brinkman flow model to characterize the rarefaction effect. We find a linear dependence on size of $\mu_{(h)eff}$ from the experiment results, which agrees with the behaviors of rarefied gas. With the obtained linear factor, an explicit expression for κ_{eff} of nanosystems is proposed, which is convenient to use and predicts κ_{eff} well for different geometries like films and wires. It shows that even in sub-100 nm systems the Darcy term still takes a considerable part of the whole resistance, which is neglected in the phonon hydrodynamics.

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