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Gas-Phonon Interaction Model for Subcontinuum Thermal Transport Simulations

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Abstract. Subcontinuum thermal transport problems such as the contact thermal resistance of semiconductor-gas interactions may play an important role in micro/nano-scale devices. In present work, a gas-phonon interaction modeling approach is suggested based on Boltzmann transport equations. Verification has been conducted by comparisons with asymptotic analytical solutions as well as previously reported numerical results and experimental data. Thermal transpiration in nano-sized channels and thermal resistance of nano-sized constrictions has been studied using the current model. Thermal transpiration is the main mechanism for temperature driven pumps in nano/micro-devices. In order to maintain higher temperature ratio between the two ends of the gas path (capillaries), the choice of membrane material is very important, and the gas-solid interaction must be understood. It is shown from the calculations that the temperature gradient, capillary geometry, gas/solid Knudsen conditions, and the gas/solid thermal conductivity ratio are all responsible for the over-all compression efficiency. Heat transfer across mesoscopic constrictions poses a similar gas-phonon coupling problem. Simulation shows that the analytical solution applies to limiting cases where the gas gap can be taken as a thin-film insulator. However, the heat flux through the gas thermal path may become a significant contributor for smaller gas phase Knudsen conditions.

Keywords: Interface thermal transport, BTE, rarefied gas dynamics.

PACS: Replace 47.45.Gx, 47.61.Cb, 51.20.+d, 51.90.+r

INTRODUCTION

Thermal transport at the nanoscale has become the focus of much research in recent years because of its applications to nano-electronics, NEMS and MEMS, nano-biological devices and many other nanotechnologies. In many of these applications, thermal transport processes in the nanostructure are strongly influenced by heat losses to a surrounding gas phase. In semiconductors and dielectrics, heat transfer is primarily by phonons, which are quanta of lattice vibrations [1]. When the phonon mean-free-path (~ 260 nm for crystalline silicon at room temperature) is comparable to the characteristic scale of temperature gradients, the classical macroscale heat transfer theory based on Fourier law breaks down [2] and the thermal transport in the solid phase can be more accurately described by the Boltzmann transport equation (BTE) for phonon propagation and scattering [3]. Similar treatment is required for molecular heat transfer in the gas phase at large Knudsen numbers (Kn) [4]. The coupling between solid and gas phase heat carriers play an important role in a multitude of current technological applications, such as thin films, thermal atomic force microscopy and microelectronics cooling. In the current work, we focus on two specific problems: thermal transpiration in nano-sized channels and thermal resistance of nano-sized constrictions. Thermal transpiration is the main mechanism in Knudsen compressors [5]. Based on original ideal [6], Vargo and Muntz et al [7] have worked out the modern version of this thermal-driven gas pump. However, it is noticed that the overall performance of such pumps highly depends on the interface interactions between gas and the membranes [8]. For thermal resistance of submicron constrictions, the most important issue is again the gas-phonon coupling at contact surfaces [9]. In the next sections, governing equations, interface/boundary treatments and numerical methods will be described, following by the results and discussion on the two target problems using the proposed gas-phonon BTE solver in details.

MODELS AND NUMERICAL METHODS

Governing Equations

For the gas phase, the steady state Boltzmann transport equation with a simplified collision operator is, [10]:

$$\mathbf{v} \cdot \nabla(f) = \frac{f_0 - f}{\tau} \quad (1)$$

where $f = f(\mathbf{x}, \mathbf{v})$ is the velocity distribution function, $\mathbf{x}$ refers to the physical space, $\mathbf{v}$ is the molecular velocity space, and $1/\tau$ is the collision frequency. In the standard Bhatnagar-Gross-Krook (BGK) model, f_0 is the local equilibrium Maxwellian distribution, $f_0 = f_M = n/(2\pi RT)^{3/2} \exp(-\mathbf{v}'^2/2RT)$, where $\mathbf{v}' = \mathbf{v} - \mathbf{v}_0$ is the thermal velocity, and $\mathbf{v}_0$ is the average flow velocity. In the ellipsoidal statistical (ES) model, f_0 is the local anisotropic Gaussian distribution:

$$f_0 = f_G = \frac{n}{\sqrt{(2\pi)^3 \det[\lambda_{ij}]}} \exp(-[\lambda_{ij}]^{-1} v_i v_j), \quad \lambda_{ij} = \frac{1}{Pr} RT \delta_{ij} + \left(1 - \frac{1}{Pr}\right) \frac{p_{ij}}{\rho} \quad (2)$$

where p_{ij} is the pressure tensor, and Pr is the Prandtl number ($Pr=0.67$ for monatomic molecules). For two-dimensional problems, reduced distribution functions f_1 and f_2 [11] are used to offset computational cost.

For the solid phase, a similar Boltzmann equation based on energy density can be written as [3]:

$$\mathbf{v}_g \cdot \nabla(e'') = \frac{e^0 - e''}{\tau} \quad (3)$$

where $e''(\mathbf{x}, \mathbf{v})$ is the net energy density of all phonon groups at position $\mathbf{x}$ and in wave-vector direction $\mathbf{v}$ in all polarizations, and $e^0(\mathbf{x})$ represents the angular average of $e''(\mathbf{x}, \mathbf{v})$, $e^0(\mathbf{x}) = 1/4\pi \sum (\int_{\Omega} e'' d\Omega)$. The gray-BTE model treats phonons of all polarizations and wave vectors as having the same group velocity v_g with a single relaxation time τ . The group velocity v_g is usually chosen to be the dominant velocity of the major phonon group at the temperature of interest. Once v_g is chosen, τ can be calculated from known bulk thermal conductivity, $k_{ph} = C_p v_g^2 \tau/3$.

Macroscopic quantities of interest can all be expressed in terms of the corresponding phase distribution functions. In particular, temperature T and heat flux $\mathbf{Q}_i$ can be written as:

$$T_{gas} = \frac{1}{3Rn} \cdot \int_{-\infty}^{\infty} \mathbf{v}'^2 f \cdot d\mathbf{v}, \quad T_{ph} = \frac{4\pi}{C_p} e^0 + T_{ref} \quad (4)$$

$$\mathbf{Q}_{i,gas} = \frac{m}{2} \cdot \int_{-\infty}^{\infty} \mathbf{v}'_i \mathbf{v}'^2 f \cdot d\mathbf{v}, \quad \mathbf{Q}_{ph} = \int_{-\infty}^{\infty} \mathbf{v}_g e'' \cdot d\mathbf{v} \quad (5)$$

Gas-phonon Interactions and Boundary Conditions

At the gas-phonon interface, conservation of mass, momentum and energy must be satisfied. The net energy flux from the gas phase is balanced by that from the phonon part. In each phase, there are two components for the energy flux, in particular, those due to incident and reflected molecules and phonons. Using Maxwell's specular-diffusive model with an accommodation coefficient, $\sigma_T = (E_{inc} - E_{refl})/E_{inc}$, the energy balance at gas-phonon interface can be imposed as follows [12]:

$$\sigma_{T,ph} [Q_{ph}(e^0, \mathbf{v} \cdot \mathbf{n}_{ph} > 0) + Q_{ph}(e'', \mathbf{v} \cdot \mathbf{n}_{ph} < 0)] = \sigma_{T,g} [Q_g(f_1^0, f_2^0, \mathbf{v} \cdot \mathbf{n}_g > 0) + Q_g(f_1, f_2, \mathbf{v} \cdot \mathbf{n}_g < 0)] \quad (6)$$

$$e''_{\mathbf{v} \cdot \mathbf{n}_{ph} > 0} = e^0_{\mathbf{v} \cdot \mathbf{n}_{ph} > 0} = \frac{C_p}{4\pi} (T_w - T_{ref}), \quad \nabla e''_{\mathbf{v} \cdot \mathbf{n}_{ph} < 0} \cdot \mathbf{v} = 0; \quad f_{1,\mathbf{v} \cdot \mathbf{n}_g > 0}^0 = f_{1,Maxwellian}^0, \quad f_{2,\mathbf{v} \cdot \mathbf{n}_g > 0}^0 = f_{2,Maxwellian}^0 \quad (7)$$

where $\mathbf{v} \cdot \mathbf{n}_{ph} < 0$ refers to outgoing directions from the solid phase into the gas, and $\mathbf{v} \cdot \mathbf{n}_{ph} > 0$ refers to outgoing directions from the gas phase domain; a similar definition is applied to $\mathbf{v} \cdot \mathbf{n}_g$.

Numerical Method

A computer code has been developed to solve the coupled gas-phonon interaction problem based on the non-dimensional form of the governing equations shown above. As we only consider steady problems with negligible external forces, the normalization analysis for equation (1) will only involve one dimensionless parameter, i.e. the Knudsen number, $Kn = \lambda/L$. In the two-dimensional discrete ordinate method, we have applied Cartesian coordinates in the physical space and polar coordinates in the velocity space. The set of discretized governing equations have been solved using first and second-order upwinding finite volume method with sixteenth-order Gauss-Hermite half-range quadrature [13] applied to the integration over the velocity magnitude. In ESBGK, a Newton's algorithm was applied to obtain the values of the local anisotropic Gaussian that strictly enforce mass, momentum and energy conservations.

Grid convergence studies have been carried out to determine the sensitivity to discretization of both physical and velocity spaces. For Kn approaching the free molecular limit for gas or the ballistic limit for phonons, a coarse mesh is sufficient since the intermolecular or inter-phonon collisions are less important compared to boundary scattering. For Kn close to the sub-continuum limit, a finer mesh is required to capture the gradients due to collisional relaxation, and to resolve sharp near-wall gradients. For example, for micro/nano-channels with large length-to-height ratio, it may be necessary to apply extrapolations of coarse-mesh solutions as initial conditions to reduce computational cost.

Verification has been performed by comparing gas phase Fourier flow (figure 1) with the data from Wadsworth [14], gas phase Couette flow with analytical solutions in the slip regime [4], and phonon heat transfer (figure 2) with analytical solutions provided in reference [15].

FIGURE 1. Gas phase thermal transportation compared with experimental data [14]. $\rho_{norm} = \rho' \rho(L_{norm}=0.5)$.

FIGURE 2. Phonon gray-BTE model compared with analytical solution [15]. $T_{norm} = (T - T_L)/(T_H - T_L)$.

RESULTS AND DISCUSSION

Thermal Transpiration in Nano-sized Capillaries

In the present work, a single stage Knudsen compressor is simulated. As shown in figure 3, two reservoirs with single-species nitrogen are connected to the two-dimensional capillary and are separated from each other by solid bulk domains. In a typical configuration, each chamber has a finite length L_{ch} and a height H_{ch} , and the channel has a length L and a height H . The left reservoir is maintained at a higher temperature, T_H , through the imposition of fixed wall boundary conditions; the other one is maintained at a lower temperature, T_L , in the same way. The system is closed, which corresponds to the final state of Knudsen compressors. Initially, there is no pressure gradient, and the flow (nitrogen with $\mu = \mu_{ref}(T/T_{ref})^{\mu_0}$) is driven by the temperature gradient, moving from the cool end to the hot one. Then, a pressure gradient builds up gradually, which induces a reverse flow against the transpiration flow. Finally, the system achieves a steady state consistent with its initial conditions with constant temperature and pressure gradients in the two reservoirs. At the steady state, there will be no net flow as the thermal creep effects are balanced by the thermal-molecular pressure effects. One can relate the final pressure and temperature at both channel ends as

$(P_2/P_1) = (T_2/T_1)^\gamma$ [16]. The power γ is influenced by the Knudsen number. In the free-molecular regime, there is experimental and theoretical work done by Reynolds considering very low pressure, [17]. Under this circumstance, the same number of molecules must enter the channel from each reservoir, which gives the following relationship: $(P_2/P_1) = (T_2/T_1)^{0.5}$, i.e. $\gamma_{FM} = 0.5$. In continuum limit, there will be no pressure gradient no matter how large the temperature gradient, and $\gamma_{cont} = 0$. In the present work, we are interested in the slip and transitional flow regimes that demand a numerical solution of the Boltzmann equation, with γ between 0 and 0.5. A list of selected cases with specific conditions is shown in table 1. Unless specified, all parameters are the identical to those in the typical case marked by *; the same is applied to table 2 in the next section.

It has been discussed in reference [8, 11] that the surface temperature distribution may have a strong influence on a open system with no pressure gradient in reservoirs. Here we also examine interface effects for the closed system by comparing results from uncoupled and coupled simulations. In the uncoupled case, only the gas phase is calculated and the capillary wall temperature profile is specified apriori as linear, varying from T_H to T_L . In coupled cases, both gas and solid phases are calculated simultaneously using the gas-surface interaction model described above. Temperature and velocity fields are found to be strongly affected by the coupling (figure 3-4). The capillary wall temperature gradient computed in the coupled case is found to be slightly lower than that for the linear case due to the use of aerogel in the solid domain, the Kn of which is finite. Since the typical thermal conductivity of aerogel is about $0.02 W \cdot m^{-1} K^{-1}$ [8], it helps maintain the temperature gradient across the capillary with minimum energy consumption. For k^* less than unity ($k_g < k_{ph}$), increasing gas phase Knudsen number will have more impact on improving the compression efficiency (indicated by larger γ), as shown in figure 5 and table 1 (case 5), compared to increasing phonon phase Knudsen number (table 1, case 6).

FIGURE 3. Temperature fields and streamlines. $T_{norm} = (T - T_L) / (T_H - T_L)$, $Kn_g = 5.1$, $Kn_{ph} = 3.0$, $k^* = 0.18$. Top: uncoupled; Bottom: coupled ($T_{solid,w} = 306 \sim 593 K$).

FIGURE 4. Temperature fields and streamlines (totally coupled). $T_{norm} = (T - T_L) / (T_H - T_L)$, $Kn_g = 5.1$, $Kn_{ph} = 3.0$. Top: $k^* = 1.8$ ($T_{solid,w} = 419 \sim 481 K$); Bottom: $k^* = 0.18$ ($T_{solid,w} = 445 \sim 453 K$).

FIGURE 5. Kn_g effects on temperature and pressure distributions. $T_H/T_L = 2$, $Kn_{ph} = 3.0$, $k^* = 0.18$.

TABLE 1. Summary of thermal transpiration results.

Variations	T_d/T_{in}	$u_o, m/s$	P_d/P_{in}	γ
1. Typical coupled case*	1.646	0.26	1.218	0.396
2. $T_H/T_L = 1.5$	1.342	0.15	1.119	0.382
3. $T_H/T_L = 1.1$	1.072	0.03	1.026	0.367
4. $L/H = 10$	1.782	0.07	1.245	0.379
5. $Kn_g = 1.0$, $Pr = 0.67$	1.749	0.26	1.252	0.401
6. $Kn_g = 5.1$, $Pr = 0.67$	1.795	0.56	1.146	0.233
7. $Kn_{ph} = 30.0$	1.753	0.39	1.249	0.396
8. $Kn_{ph} = 30.0$	1.552	0.31	1.186	0.388

* $L/H = 5$, $L_{ch}/H_{ch} = 1$, $T_H/T_L = 2$, $Kn_g = 5.1$, $Kn_{ph} = 3.0$, $k^* = 0.18$, $Pr = 1.0$.

Thermal Resistance of Nano-sized Constrictions

It has been shown in the thermal transpiration calculations that the gas-surface interaction can play an important role in the overall thermal transport. In carbon nanotube (CNT) thermal interface materials (TIM), the constricted interfaces formed between the CNT's are the bottleneck for the overall heat transfer as the nanostructure itself is

highly conductive [18]. In this section, we will apply the presented gas-phonon numerical model to study the thermal resistance of a nano-sized constriction. In the free molecular limit, the gas phase heat flux can be neglected, and the analytical solution for phonon thermal resistance in ballistic limit is given by: $R_{analy} = v_g C_p / 4$, and $Q_{analy} = R_{analy} \Delta T$ [9].

In simulations, though the gas phase has a high Kn number, its thermal conductivity is small but finite. In figure 6, it is shown that by increasing the ratio of L_{solid}/H_{solid} the heat flux in the direction of the temperature gradient gradually approaches the analytical limit. Hence, the heat flux normal to the temperature gradient will matter if the constriction has small length-to-height ratio. Knudsen conditions for the gas and phonon phases are also important in analyzing the overall effective thermal resistance through constrictions. It is known that the heat flux for the free molecular flow of a gas is proportional to the pressure [4]. The thermal resistance of the gas path is much larger than that of the solid contact in cases shown in figure 7, and the main heat transfer pathway is solely due to phonon transport through the constriction. For smaller gas Knudsen numbers, the heat transfer through gas gaps increases and may become a major contributor to the total heat flux, which can be seen clearly from the heat flux contours shown in figure 8. A summary of the heat flux through the constriction and gas gap for selected cases is listed in table 2.

FIGURE 6. Heat flux dependence on constriction size and temperature gradient. $Kn_{ph}=2.6$, $Kn_g=800$, $k^*=0.18$.

TABLE 2. Summary of thermal resistance results.

Variations	Q_{yph}/Q_{tot}	Q_{yg}/Q_{tot}	Q_{tot}/Q_{analy} [9]
1. Typical case*	0.9197	0.0251	0.8088
2. $L_{solid}/H_{solid}=4$	0.9644	0.0109	0.9202
$L_{solid}/H_{solid}=6$	0.9787	0.0064	0.9325
$L_{solid}/H_{solid}=8$	0.9859	0.0043	0.9373
3. $Kn_{ph}=2.6$	0.9274	0.0178	1.9590
$Kn_{ph}=0.26$	0.9295	0.0178	9.4662
4. $Kn_{ph}=2.6, Kn_g=8$	0.0951	0.8914	0.3952
$Kn_{ph}=0.26, Kn_g=8$	0.0947	0.9414	0.3867

* $L_{solid}/H_{solid}=2$, $T_H=310K$, $T_L=300K$, $Kn_{ph}=26$, $Kn_g=800$, $k^*=0.18$.

FIGURE 7. Kn effects on heat flux. $Q_{y,norm}=Q/Q_{analy}$, $T/T_L=10/300$, $Kn_g=800$, $k^*=0.18$.

Left: $Kn_{ph}=0.26$, Right: $Kn_{ph}=2.6$.

FIGURE 8. Kn effects on heat flux. $Q_{y,norm}=Q/Q_{analy}$, $T/T_L=10/300$, $Kn_g=8$, $k^*=0.18$.

Left: $Kn_{ph}=0.26$, Right: $Kn_{ph}=2.6$.

CONCLUSIONS

A coupled gas-phonon Boltzmann solver has been developed and applied to the study of sub-micron solid-gas thermal transport. Validation has been carried out by comparing simulation results with experiments and analytical solutions for gas phase Fourier flow and Couette flow as well as for phonon thermal transport problems. In a closed thermal transpiration system, a pressure difference builds up when there is a temperature difference between the chambers. The process is found to be affected by many factors such as reservoir and channel geometries (length-to-

height ratios), gas and phonon thermal conductivities, and Knudsen conditions. It has been shown that the thermal coupling at interfaces becomes important when the solid separating the reservoirs has a low thermal conductivity and a high Knudsen number. The role of gas-solid coupling in the overall thermal resistance of nano-sized constrictions has also been studied. The heat flux normal to the temperature gradient cannot be neglected if the constriction geometry is with small length-to-height ratio. The Knudsen number of the gas gap is also found to play an important role in the determining the primary heat transfer path.

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