One-dimensional thin-film phonon transport with generation

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ABSTRACT: The Boltzmann transport equation is often used for non-continuum transport when the mean free path of phonons is of the order of device sizes. One particular application involves heat generation in electronic devices. In a highly scaled MOSFET, for example, the majority of the heat is produced in a localized region immediately below the gate on the drain side. The size of this generation region is often smaller than the mean free path of phonons, which demands the BTE for transport calculations. Using a one-dimensional BTE and diffusion equation, a comparison between the continuum and non-continuum models is made. The focus of this comparative study is the behavior of each model for various Knudsen numbers, while actual devices and material properties are ignored. Results suggest that non-continuum distributions are similar to continuum distributions except that the jump condition at the boundary results in slightly larger magnitude in energy. In particular, ballistic transport minimizes the distribution but increases the jump at the boundary.

1 INTRODUCTION

Use of non-continuum models for thermal transport of highly scaled devices is usually justified by comparing the mean free path of phonons to characteristic device dimensions. The ratio of mean free path (l) to device size is often termed the thermal Knudsen number, and is defined as $\mathrm{Kn} = l/L$. If Kn is near or above unity, then non-continuum effects should be considered when calculating transport. Transport for devices where $\mathrm{Kn} \ll 1$ approaches that of common continuum models such as Fourier's law and the diffusion equation.

Non-continuum effects are very clearly seen by examining a one-dimensional film with an imposed temperature difference. The temperature distribution in such devices with large Kn exhibit a jump at the boundaries and a smaller slope compared to the continuum limit. Many researchers use this case to validate more complex simulations and so these results appear in numerous publications (Majumdar, 1993; Klitsner et al., 1988; Zhang et al., 2002; Narumanchi et al., 2004; Escobar et al., 2006). In fact, this canonical plot is repeated in the results section as a validation for the non-continuum formulation in the present work.

The pressure to reduce the size of microelectronic devices has largely driven the trend toward nanoscale science and technology. In fact, most of the fabrication and characterization capabilities were developed for microelectronic devices. Consequently, it is no surprise that microelectronic de-

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vices and materials are particularly interesting to study in terms of thermal transport (Cahill et al., 2003). The majority of thermal modeling of microelectronic materials has been relegated to thermal conductivity prediction of reduced-scale structures (Zeng and Chen, 2003; Prasher, 2003) or detailed examination of dispersion effects (Chung et al., 2004). Likewise, thermal experiments on nanoscale devices involves mostly thermal conductivity measurements (Asheghi et al., 1998, 2002; Cahill et al., 2002). Nevertheless more effort is being devoted to actual transport including generation of thermal energy at reduced scales recently. Here microelectronics provides an ideal system to study because thin-film devices such as SOI MOSFETs provide reduced scales with highly localized heating (Raman et al., 2003; Lai and Majumdar, 1996; Raha et al., 1997). This particular application is significant because the continued scaling of practical CMOS devices is limited not by manufacturing technology, but by heat removal by production technologies (i.e. air cooling) (Semiconductor Industry Association, 2003).

The argument for using non-continuum solutions to study heat generation and dissipation in highly scaled microelectronic devices is similar to the argument for transport across thin films. If the generation region is small compared to the mean free path of phonons then non-continuum models are required (Sverdrup et al., 2001). This is often referred to as the *hot-spot problem*. It has been suggested that the localization of the generation results in an increase in local energy (Ju and Goodson, 1999; Pop et al., 2001). However, if we consider that transport is largely ballistic in the region of generation for small generation regions, then the phonons will escape the generation region without scattering leaving the localized region unchanged in terms of energy. This premise is not precisely valid because of the way we calculate energy and define temperature in non-continuum systems, but conceptually the scenario is not inconceivable. Using this logic, the localization of the energy generation must be at least twice as large as the mean free path of phonons even if the region where generation occurs is a point. The present work represents a preliminary attempt to understand this hypothesis in terms of a limited number of parameters.

A non-continuum analytic model of a one-dimensional system with generation is developed to help understand how non-continuum effects manifest themselves in devices with generation. The current work investigates the difference between non-continuum and continuum models to identify where continuum models break down.

2 THEORY

2.1 Non-continuum

The derivation of the steady-state blackbody emissive power distribution for various Knudsen numbers (Kn) without generation is well known (Chen et al., 2005). However, the development is largely repeated here with emphasis on the non-homogeneous generation term because this solution is central to the discussion. The intensity formalism follows that found in many radiation texts (Modest, 2003) due to the similarity between phonon and photon transport (Majumdar, 1993). The intensity is essentially a moment of the distribution function.

The steady-state Boltzmann transport equation for phonons is written in terms of an intensity using the relaxation time approximation as

$$\mu v \frac{dI}{dx^*} + \frac{I - I_0}{\tau} = g^* \quad \Longrightarrow \quad \mu \frac{dI}{dx} + I - I_0 = \tau g^* = g, \tag{1}$$

where the coordinate x is non-dimensionalized with the quantity $v\tau$ such that the real spatial coordinate $x^* = v\tau x$. $\mu = cos\theta$ is the direction cosine, and I_0 is the equilibrium intensity. In the foregoing analysis the magnitude of the phonon group velocity v and scattering rate $1/\tau$ are assumed constant. This approximation is equivalent to the gray assumption, so the intensity is independent of frequency.

The combined parameter $l = v\tau$ is the mean free path of phonons. The generation rate g is a source term that represents an increase in local intensity resulting from electron phonon scattering, for example. Therefore, the form of g is initially treated as arbitrary, but will have specific known forms for subsequent analysis.

The solution to the governing equation is given as a combination of positively moving phonons and negatively moving phonons as

$$I^+(x,\mu) = C_1 \exp\left(-\frac{x}{\mu}\right) + \int_0^x \left[\frac{I_0(x')}{\mu} + \frac{g(x')}{\mu}\right] \exp\left(-\frac{x-x'}{\mu}\right) dx' \qquad \mu > 0, \quad (2)$$

$$I^-(x,\mu) = C_2 \exp\left(-\frac{x-L}{\mu}\right) + \int_L^x \left[\frac{I_0(x')}{\mu} + \frac{g(x')}{\mu}\right] \exp\left(-\frac{x-x'}{\mu}\right) dx' \qquad \mu < 0. \quad (3)$$

For now, the integration constants (C_1 and C_2) will be left as unknown constants but will be determined from assigned emissive power at the boundaries of the film. Note that these constants are independent of the generation or the intensity distribution within the medium. This is a result of the directionality and independence of the two phonon systems. Note that the generation $g(x)$ is an arbitrary function of x as is the equilibrium intensity $I_0(x)$, and both are treated as a non-homogeneity in the equation. The two terms, however, represent different mechanisms and will be treated differently at a later step.

The heat flux is obtained from the intensity as an integration over the hemisphere yielding

$$J(x) = J^+(x) + J^-(x) = 2\pi \int_0^1 \mu I^+(x,\mu)\, d\mu + 2\pi \int_0^{-1} \mu I^-(x,\mu)\, d\mu. \quad (4)$$

Each term on the right hand side can be expanded by plugging equations 2 and 3 into equation 4 such that

$$\begin{aligned} J^+(x) &= 2\pi C_1 \int_0^1 \mu \exp\left(-\frac{x}{\mu}\right) d\mu + 2\pi \int_0^x [I_0(x') + g(x')] \int_0^1 \exp(-\frac{x-x'}{\mu})\, d\mu\, dx', \\ &= 2\pi C_1 \mathrm{E}_3(x) + 2\pi \int_0^x [I_0(x') + g(x')] \mathrm{E}_2(x-x')\, dx', \quad \text{and} \qquad (5) \\ J^-(x) &= 2\pi C_2 \int_0^{-1} \mu \exp\left(-\frac{x-L}{\mu}\right) d\mu + 2\pi \int_L^x [I_0(x') + g(x')] \int_0^{-1} \exp(-\frac{x-x'}{\mu})\, d\mu\, dx', \\ &= 2\pi C_2 \mathrm{E}_3(L-x) + 2\pi \int_L^x [I_0(x') + g(x')] \mathrm{E}_2(x-x')\, dx'. \qquad (6) \end{aligned}$$

The exponential integral $\mathrm{E}_n(x)$, along with identities and properties involving this special function can be found in Abramowitz and Stegun (1972). Now the total heat flux is the sum of each component. In the absence of generation, the heat flux is constant across the domain to conserve energy, or $dJ(x)/dx = 0$. With generation, however, the heat flux must satisfy energy conservation as

$$\frac{dJ(x)}{dx} = g(x). \quad (7)$$

This condition is satisfied by summing equations 5 and 6 and differentiating.

$$\begin{aligned} C_1 \mathrm{E}_2(x) + \int_0^x [I_0(x') + g(x')] \mathrm{E}_1(x-x')\, dx' - 2[I_0(x) + g(x)] \\ + C_2 \mathrm{E}_2(L-x) - \int_L^x [I_0(x') + g(x')] \mathrm{E}_1(x'-x)\, dx' = -\frac{g(x)}{2\pi}. \quad (8) \end{aligned}$$

The foregoing expression is a non-homogeneous integral equation in $I_0(x)$ if we assume $g(x)$ is known. We can use any number of numerical integration approaches to approximate the solution.

2.2 Continuum

The Boltzmann solution for $I_0(x)$ (equation 8) should recover the continuum solution for large domains. The one-dimensional heat diffusion equation provides a temperature distribution for continuum systems that can be compared to the non-continuum results. The diffusion equation with generation is given as

$$\frac{d^2T}{dx^2} = -G(x), \tag{9}$$

The solution depends on the functional form of the generation term $G(x)$. In the case of no generation, the solution reduces to a line and the integration constant are given as a combination of the boundary conditions. Although the two constants may be the same as the two boundary constants in the non-continuum case for no generation, in general they are dependent on the generation unlike the non-continuum constants.

For the case of a constant generation, the solution is obtained via direct integration

$$T(x) = B_1 + (B_2 - B_1)\frac{x}{L} + \frac{G}{2}(xL - x^2), \tag{10}$$

where the first two terms represent the linear no generation component for left and right boundary temperatures of B_1 and B_2 respectively.

The continuum solution for a delta pulse is simply the Green's function solution for the LaPlacian with a Dirac delta source.

2.3 Model comparison

When comparing the continuum solution to the non-continuum solution we need to be cognizant of the following issues.

1. The coordinate x was defined in terms of the mean free path. We are using this same normalized coordinate for the continuum solution even though this quantity does not have any real physical significance in the continuum limit. However, we intend to keep this structure because we want to compare the two models despite the presumed lack of applicability of the continuum model at large Kn.

2. The definition of "temperature" in the two cases is fundamentally different. In general, we regard equilibrium energy and temperature as related, so the real question is whether the definition of equilibrium energy is equivalent for both systems. For non-continuum situations, the quantity I_0 represents an average energy of the left moving phonons and the right moving phonons emitted from their respective boundaries and the medium. It is *not* the equilibrium energy of the phonon system at any point since equilibrium does not exist. In the continuum limit, though, I_0 reduces to the continuum equilibrium energy. The difference between the definitions, though is exactly what we intend to exploit to identify non-continuum effects.

3. The generation in the continuum and non-continuum model have the same functional form, but are different quantities. If we want to compare the response from each model, we need to ensure that identical amounts of energy are added to the system for each model. We can achieve this by assuming a scaling factor so that $G(x) = f_g g(x)$. To determine this factor we must ensure that the same amount of total energy is injected into the system as described by each model. Therefore, the heat flux at the boundaries should be the same for each model.

4. The boundary designation in each model is also not necessarily equivalent. In both cases, the boundaries are considered to be thermalizing boundaries. In the continuum model this

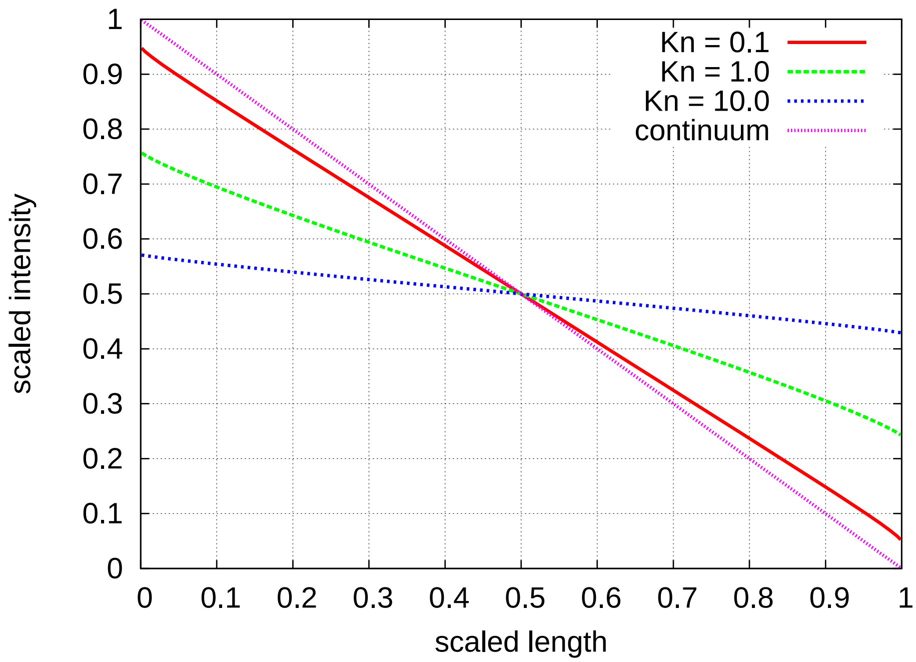

Figure 1: Steady-state, one-dimensional solution without generation for various Knudsen numbers compared to the continuum solution.

means that the temperature is specified explicitly. In the non-continuum model, we specify the equilibrium (black body) emissive power at a boundary emitted *into* the system.

5. The two models do not depend on the same material properties. The continuum model requires the thermal conductivity, whereas the non-continuum model requires the phonon mean free path. While these two parameters are phenomenologically related, an exact relation is difficult to obtain and dependent on a number of other factors (Holland, 1963). However, we can eliminate the dependence of these parameters through suitable normalization.

3 RESULTS

The steady solution is shown in Figure 1 to demonstrate that the derivation and calculation can recover the expected behavior of transport through a thin film without generation. The jump condition at the boundary is due to the lack of interaction between opposite moving phonons. Because scattering is limited for systems whose dimensions are of the order of the mean free path or smaller (large Kn), the phonons emitted from the boundary travel ballistically across the domain where they are thermalized at the opposite boundary. The intensity plotted in Figure 1 is simply the average energy of the left and right moving phonons. As the device becomes larger (small Knudsen numbers) more scattering causes the phonons to equilibrate or assume a similar energy. In the continuum limit, both phonon systems are in equilibrium everywhere.

For both generation cases, the boundary conditions are fixed at zero so the effects of the generation can be isolated. The two types of generation examined include a constant generation across the domain and a delta function in the middle of the domain. The constant generation case would model something like an extremely thin resistor where Joule heating is responsible for the thermal generation. This case, however, does not model the hot-spot problem.

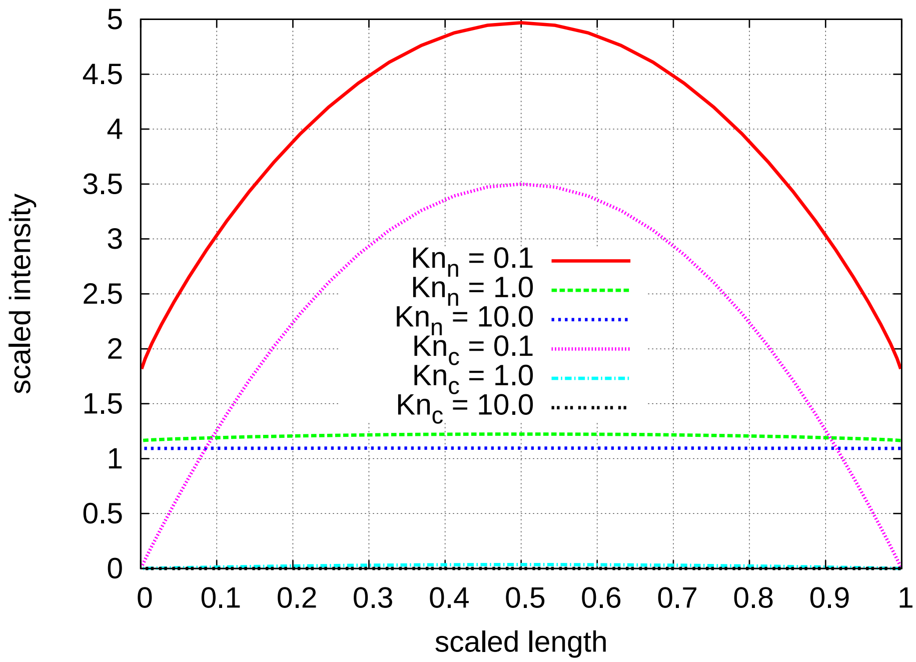

Figure 2: Steady-state, one-dimensional solution (subscript 'n') with constant generation over the domain for various Knudsen numbers compared to the continuum solution (subscript 'c'). The non-continuum solutions are easily identified as those not satisfying the zero boundary condition.

To make a fair comparison, a suitable scaling factor should be computed such that $G(x) = f_g g(x)$. We want to ensure that the same amount of energy was deposited into the system for each model. Therefore, the distribution predicted by the non-continuum model for extremely small Knudsen numbers was calculated. The scaling factor f was adjusted until the continuum solution matched to non-continuum solution. This scale factor was used for the reminder of the continuum distributions.

For constant generation, results are found in Figure 2. The shape of the distribution is very similar to the parabolic distribution of temperature found in the continuum solution. Direct comparison of the continuum solution and the non-continuum results is difficult because the appropriate scaling of the generation term is unknown. The results also demonstrate that the magnitude of the distribution grows with larger systems (small Kn). This also mirrors the behavior of a continuum system because more energy is introduced into the system as it becomes larger. Despite the zero boundary conditions, we still see a jump in the distribution. This feature is the result of ballistic phonons traveling to the thermalizing boundaries before they are equilibrated and is more prominent for large Knudsen numbers. This feature suggests that a non-continuum model might be sufficient to predict energy distribution, but jump conditions at the boundary, which dictate the ultimate energy magnitude, can not be recovered with a continuum model.

The pulse generation case models a situation more closely aligned with a hot-spot problem. Figure 3 shows similar features as the constant generation case. Note that mathematically, the distribution at the pulse is infinite. However, a small distance from the pulse, the continuum model is recovered. In fact the continuum model matches the results well for all Knudsen numbers except for the jump condition. Again, for large Knudsen numbers the ballistic phonons do not contribute appreciably to the distribution except to increase the jump condition.

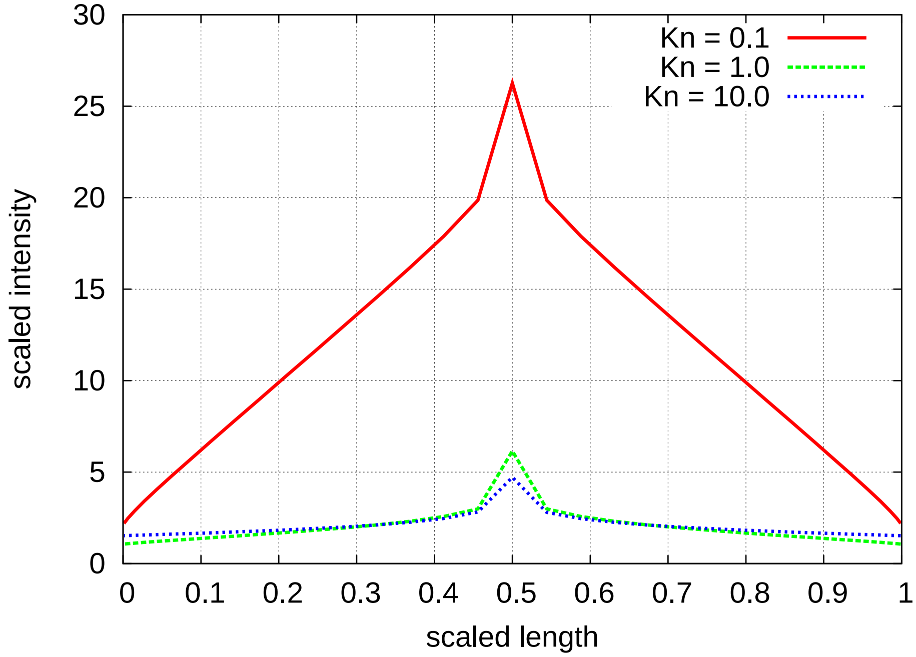

Figure 3: Steady-state, one-dimensional solution with a generation spike in the middle of the domain for various Knudsen numbers. The spike is a numerical artifact of trying to resolve the infinity and does not necessarily represent the physical distribution.

4 CONCLUSIONS

Non-continuum models with generation are similar to continuum models in functional form for all Knudsen numbers. The difference occurs in the jump condition at the boundary. For large Knudsen numbers, the jump condition is larger than the overall difference between the minimum and maximum temperature. However, where non-continuum effects are prominent, the near-ballistic transport removes the generated phonons to the thermalized boundaries without increasing the average local energy. This feature is essentially a result of the standard definition for temperature in non-equilibrium regimes. This result, however, suggests that the significance of non-continuum effects with generation deserves additional investigation, particularly in the jump condition.

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