BOLTZMANN SOLVER FOR PHONON TRANSPORT

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ABSTRACT
Boltzmann Transport Equation is solved numerically to model phonon transport in a sub-continuum domain in order to study heat transfer in thin film semiconductors. The phonon distribution function is modified to get an Energy equation from the Boltzmann Transport Equation. Gray form of the Energy equation is solved in the Relaxation time approximation to get the Phonon Energy Density distribution. The phonon group velocity and the relaxation times are obtained using other methods. Structured Finite Volume Method is used to discretize the Energy equation and a recursive solution procedure is used to solve it. Temperatures in the domain are obtained by assuming statistical equilibrium. The temperature profiles and heat fluxes for different acoustic thicknesses agree with theoretical radiation results by Heaslet and Warming. Silicon bulk thermal conductivity is reproduced under the acoustically thick limit. Boundary scattering and confinement effects are studied by working with specularity and confinement parameters.

NOMENCLATURE
\( f \) phonon distribution function
\( \nu_g \) phonon group velocity
\( \vec{k} \) phonon wave vector
\( \tau_{\text{eff}} \) effective relaxation time
\( \omega \) phonon frequency
\( \hbar \) modified Planck’s constant
\( \omega^e \) phonon energy density
\( D(\omega) \) phonon density of states
\( k \) Boltzmann constant
\( \vec{s} \) unit direction vector
\( \vec{r} \) position vector
\( t \) time
\( e^o \) angular averaged phonon energy density
\( C \) specific heat
\( T_{\text{ref}} \) reference temperature
\( \Delta\Omega \) control angle

INTRODUCTION
During the last 10 years heat conduction at the sub-micron level has received increasing attention. One of the reasons for this has been the continued and aggressive scaling of micro-electronic devices bringing into sharp focus thermal among other issues [1]. The problems related to self-heating in microelectronic devices have exacerbated for example in some of the new device designs like SOI(Silicon On Insulator) and others involving low conductivity semiconductors and dielectrics. The thermal management of these devices has thus become critical to device performance. It has been observed that at the sub-micron level the classical Fourier model for heat conduction is not only suspect but in fact gives grossly erroneous results. This is not particularly surprising given the fact that the Fourier relation is an empirical relation obtained from experimental observations at large scales rather than from any concrete physical principles. Thermal conductivity is not a material property and it can depend on the geometry and length scales of the sample [7]. Heat conduction at small scales is of critical importance in not one but many areas such as microelectronics, thin-films, superlattices, nanomaterials, short pulse laser heating, etc. [5]. Heat in solids is carried by electrons and phonons. Electrons are the predominant carriers in conductors while phonons are responsible for most the transport in semiconductors and insulators. Phonons are quantized lattice vibrations [6]. Though phonons are inherently wavelike we can think of phonons as particles when the domain of interest is larger than the phonon wavelength. This is the case in most of the devices at the sub-micron level. The

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\[ C \] specific heat
\[ T_{\text{ref}} \] reference temperature
\[ \Delta\Omega \] control angle
Boltzmann transport equation employs the particle-like nature of phonons to model heat transfer at small scales. When the length of the domain of interest is of the order of mean free path of the phonons or the time scale of interest is of the order of relaxation time of the phonons, the Fourier model of conduction cannot be applied. As long as the domain of interest is larger than the wavelength of the phonons Boltzmann transport equation with Relaxation time approximation can be used to model phonon transport. Under these conditions the phase coherence effects and other wavelike properties of the phonons are not important [1]. We propose a structured finite volume method to solve the Boltzmann equation in the relaxation time approximation to study heat transfer in sub-micron domains. The Boltzmann transport equation is a statement of conservation of the phonon distribution function. The Boltzmann transport equation can be converted into an energy equation which solves for the phonon energy density. Phonons are characterized by parameters like polarization, frequency and group velocity. The dispersion curve gives the relation between frequency and wave vector for a particular phonon branch and also computes the group velocity of the phonons at a particular frequency. For a particular phonon polarization more than one phonon branches can exist which can be degenerate or otherwise. The dispersion curve is obtained by modeling the lattice dynamics of a material. Different materials have different dispersion curves and they can be quite complex. Apart from propagation, phonons undergo scattering, in the domain and at the boundaries. Domain scattering is usually modeled using the relaxation time approximation, characterized by a relaxation time which is a function of phonon frequency and polarization, and material properties. For heat transfer purposes it is convenient to solve for phonon energy rather than its distribution. We can convert the Boltzmann transport equation into an equivalent Phonon Energy equation which solves for a quantity called the Phonon energy density. This quantity provides comprehensive information about how energy is carried by phonons inside the material. We will solve the Gray Phonon Boltzmann transport equation where the group velocity and scattering times are assumed independent of phonon frequency and polarization. The boundary conditions are also important for heat transfer in confined domains. An example is lateral conduction in thin films where boundary scattering is large enough to significantly affect phonon propagation. Three different kinds of boundary conditions have been modeled. Thermalizing boundaries act as energy reservoirs at a particular temperature; specular boundaries assume perfect reflection while diffuse boundaries model dispersive reflection. The Energy equation is discretized using the finite volume method. A Cartesian grid specifies the position of the phonons while a Polar grid indicates the direction of propagation. The nominally linear set of equations is solved using a recursive solution procedure employing Line-by-line TDMA algorithm. The Temperature and Heat flux results are compared with theoretical Radiation results by Heaslet and Warming, since the Radiation transport equation has a form similar to the Boltzmann transport equation with specular boundaries. The results match very well with these published radiation results. The bulk thermal conductivity of silicon is accurately predicted by the Boltzmann transport equation results. The confinement and boundary scattering results provide an insight into the effect of boundary scattering on thermal transport in thin films.

GOVERNING EQUATIONS

The general form of the Boltzmann transport equation is

\[
\frac{\partial f}{\partial t} + \vec{v}_g \cdot \nabla f + \frac{\partial \vec{k}}{\partial t} \cdot \nabla f = \left( \frac{\partial f}{\partial t} \right)_{\text{collisions}} \tag{eqn.1}
\]

Here, \( f(\vec{r}, t, \vec{k}) \) is the Phonon distribution function, which is the number of phonons at position \( \vec{r} \), at time \( t \), with wave vector \( \vec{k} \) and polarization \( p \), per unit solid angle, per unit wave number interval, per unit volume. \( \vec{v}_g \) and \( \vec{k} \) are the phonon group velocity and phonon wave vector respectively of the phonons. (eqn.1) indicates that the phonon distribution can change with time due to convection of phonons both in the real space and in the wave vector space. We will neglect the contribution of the latter term. The collision term on the right hand side of the equation denotes the change in the Phonon distribution function due to collisions between phonons. The collisions can be elastic or inelastic. When the number of collisions is very large, kinetic theory can be used to characterize the collisions in terms of effective scattering or relaxation times. The collision term
can thus be represented using the Relaxation time approximation as follows
\[
\left( \frac{\partial f}{\partial t} \right)_{\text{collisions}} = -\frac{(f - f_\infty)}{\tau_{\text{eff}}} \quad (eqn.2)
\]
Where \( f_\infty \) is the equilibrium phonon distribution given by the Bose-Einstein distribution
\[
f_\infty = \frac{1}{\exp\left(\frac{\hbar \omega}{kT}\right) - 1} \quad (eqn.3)
\]
and \( \tau_{\text{eff}} \) is the effective relaxation time of the phonons. The determination of the effective relaxation times is a separate problem and we won’t discuss it here. The Phonon distribution function can be transformed into a Phonon energy density as follows
\[
e_{\omega}^\prime = \hbar \omega D(\omega) f \quad (eqn.4)
\]
Here \( \hbar \) is the modified Planck’s constant, \( \omega \) is the phonon frequency and \( D(\omega) \) is the Phonon density of states function. The Boltzmann transport equation is transformed into an Energy equation
\[
\frac{\partial e_{\omega}^\prime}{\partial t} + \vec{\nabla} \cdot \vec{E}_{\omega}^\prime = \frac{e_{\omega}^\prime - e_{\omega}}{\tau_{\text{eff}}} \quad (eqn.4)
\]
where the phonon energy density \( e_{\omega}^\prime \) is the energy of phonons with frequency \( \omega \), at position \( \vec{r} \), at time \( t \), per unit volume, per unit frequency, per unit frequency interval and \( \vec{s} \) is the unit direction vector of propagation. Here the phonon group velocity and relaxation times are frequency dependent. We will be solving for the Steady state Gray Phonon Boltzmann transport equation, where the phonon group velocity and relaxation time will be considered independent of frequency and polarization.
\[
\nabla(\vec{s} v_{\omega} e^\prime) = \frac{e^\prime - e}{\tau_{\text{eff}}} \quad (eqn.5)
\]
e is the frequency independent Phonon energy density while \( e^\prime \) is the direction independent angular average of \( e^\prime \).
\[
e^\prime(\vec{r}, t) = \frac{1}{4\pi} \int e^\prime(\vec{s}, \vec{r}, t) d\Omega \quad (eqn.6)
\]
At equilibrium, the lattice temperature is defined as
\[
\frac{\int_{T_{\text{ref}}}^{T} C dT}{T_{\text{ref}}} = 4\pi e^\prime \quad (eqn.7)
\]
and if the specific heat is assumed constant we have
\[
T = \frac{4\pi e^\prime}{C} + T_{\text{ref}} \quad (eqn.8)
\]

**BOUNDARY CONDITIONS**

The following phonon processes can occur at the boundaries: emission, absorption, reflection, and transmission. We can think of phonon reservoirs at the boundaries which can emit and absorb phonons. The rest of the boundaries can be thought of as reflection and transmission boundaries where incident phonons undergo reflection and transmission depending on the physical characteristics of these boundaries. We will employ the following four types of boundary conditions.

**THERMALIZING BOUNDARIES**

The Boltzmann transport equation domain can be thought of as bounded by reservoirs which are in thermal equilibrium and thus have a unique temperature. These reservoirs absorb the incident phonons while they radiate phonons equally in all directions into the domain. Statistical thermodynamics gives the energy of the emitted phonons as
\[
e^\prime = e^\prime = \frac{C}{4\pi} (T_b - T_{\text{ref}}) \quad (eqn.9)
\]
where \( C \) is the specific heat of the reservoir material, \( T_b \) is the boundary reservoir temperature and \( T_{\text{ref}} \) is the reference temperature with respect to which the specific heat is defined.

**SPECULAR BOUNDARIES**

These are boundaries where phonons are assumed to undergo perfect reflection according to Snell’s law. We require phonon energy information only for directions incoming to the domain, which is
\[
e^\prime(\vec{r}_b, \vec{s}_r, t) = e^\prime(\vec{r}_b, \vec{s}_i, t) \quad (eqn.10)
\]
where \( \vec{r}_b \) is the boundary position, \( \vec{s}_i \) is the incident direction and \( \vec{s}_r \) is the reflected direction.

**DIFFUSE BOUNDARIES**

At the diffuse boundaries all the incident phonons are reflected in a perfectly diffuse manner. In order to find the energy of phonons incoming to the domain, first the...
average energy incident on the boundary is calculated using
\[ e'_{\text{inc min to boundary}} = \frac{1}{\pi} \int e' \tilde{s}, \tilde{n}d\Omega \quad (\text{eqn.11}) \]
The energy of the phonons incoming to the domain is equal to the above energy in all directions.
\[ e_{\text{inc min to domain}} = e'_{\text{inc min to boundary}} \]
\[ = \frac{1}{\pi} \int e' \tilde{s}, \tilde{n}d\Omega \quad (\text{eqn.12}) \]

**PARTIALLY SPECULAR AND PARTIALLY DIFFUSE BOUNDARIES**

Depending on the roughness and other boundary properties a fraction of the phonons can be thought of as reflecting specularly and the rest of them diffusely. The energy of the phonons incoming to the domain can then be calculated as
\[ e' = p e'_{\text{boundary, specular}} + (1 - p)e'_{\text{boundary, diffuse}} \quad (\text{eqn.13}) \]
where \( p \) is termed the specularity factor.

**NUMERICAL METHOD**

Structured finite volume method has been used to discretize the Energy equation (eqn.5). The nominally linear set of algebraic equations thus obtained are solved iteratively using the Line-by-line TDMA algorithm.

**DISCRETIZATION**

The Energy equation is solved in a 2-D rectangular domain. The domain is discretized into a structured cartesian grid as shown in Fig.1.

![Fig.1 The cartesian domain](image)

The position of the phonons is specified by the Cartesian grid. The direction of phonon propagation also needs to be specified which can be done using an angular grid. Although the problem is solved in a 2-D domain, phonons are inherently 3-D carriers so a polar grid is used as shown in Fig.2. The Cartesian domain is divided into \( I \times J \) control volumes while the angular domain is divided into \( N_\theta \times N_\phi \) control angles per octant.

![Fig.2 The Polar angular domain](image)

The position of a phonon is given by \( (x_i, y_j) \) while the direction of its propagation is given by the centroid of the control angle \( (\theta_k, \phi_l) \). The direction of propagation vector \( \tilde{s} \) is then given by
\[ \tilde{s} = \sin \theta_k \sin \phi_l \hat{i} + \sin \theta_k \cos \phi_l \hat{j} + \cos \theta_k \hat{k} \quad (\text{eqn.13}) \]
while the control angle is
\[ \Delta\Omega = \text{weight factor} \times 2 \sin \theta_i \sin \left( \frac{\Delta \theta}{2} \right) \Delta\phi \quad (\text{eqn.14}) \]

Here a weight factor of 2 is employed since we will be solving for only half of the spherical domain due to symmetry. The Energy equation (eqn.5), is discretized over the Cartesian and angular domains using the Finite volume Upwind difference scheme (UDS). The discretized set of algebraic equations are as follows
\[ a_{i,P}e_{i,P} = \sum_{nb} a_{i,nb}e_{i,nb} + b_{i,P} \]
\[ a_{i,E} = v_g \Delta y \text{Max}(-S_{x,i}, 0) \]
\[ a_{i,W} = v_g \Delta y \text{Max}(S_{x,i}, 0) \]
\[ a_{i,N} = v_g \Delta x \text{Max}(-S_{y,i}, 0) \]
\[ a_{i,S} = v_g \Delta x \text{Max}(S_{y,i}, 0) \]
\[ a_{i,P} = \sum_{nb} a_{i,nb} + \frac{\Delta x \Delta y}{\tau_{\text{eff}}} \Delta\Omega_i \]
\[ b_{i,P} = \frac{\Delta x \Delta y \Delta\Omega_i}{\tau_{\text{eff}}} e_{i,P}^o \]
\[ e_{i,P}^o = \frac{1}{4\pi} \sum_j e_{j,P}^o \Delta\Omega_j \quad (\text{eqn.15}) \]
where

\[
\bar{S} = \int_{\phi - \Delta \phi/2}^{\phi + \Delta \phi/2} \int \bar{s} \sin \theta d \theta d \phi
\]

\[
= \text{weight factor} \times \sin \phi \sin \left( \frac{\Delta \phi}{2} \right) \left[ \frac{L}{v_g} \left( \Delta \theta - \cos(2\theta) \sin \Delta \theta \right)^2 \right] \]

+ \cos \phi \sin \left( \frac{\Delta \phi}{2} \right) \left[ \frac{L}{v_g} \left( \Delta \theta - \cos(2\theta) \sin \Delta \theta \right) \right] \]

\[
\times \sin \left( \frac{\Delta \phi}{2} \right) \sin \Delta \theta \hat{k}
\]

**SOLUTION PROCEDURE**

The set of nominally linear algebraic equations (\(eqn.15\)) is solved using an iterative scheme. We have \(I \times J \times N_\phi \times N_\theta\) number of unknown variables and the same number of equations. The variables are just \(e_{i,P}\) at different positions in the domain and in different directions. Line-by-Line TDMA algorithm is used in an iterative procedure to solve the set of nominally linear algebraic equations. The solution procedure is explained in the flowchart shown in Fig.3.

**RESULTS**

In order to study the results of the Boltzmann solver, we will define a non-dimensional term called acoustic thickness

\[
\text{Acoustic thickness} = \frac{L}{v_g \tau_{\text{eff}}} \quad (\text{eqn.16})
\]

Here \(L\) is the length of the problem domain in the direction of propagation of the phonons.

**COMPARISON WITH HEASLET AND WARMING RADIATION PROBLEM**

In order to validate the Boltzmann transport equation solver, we will compare some of the results with the Haslet and Warming problem. This is a participating media radiation problem between infinite parallel plates and has a theoretical solution. The corresponding Boltzmann transport problem will have phonon transport between two thermalizing boundaries with the rest of the boundaries being specular as shown in Fig.4.

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Fig.3 The solution procedure
TEMPERATURE PROFILES

The temperatures inside the solution domain are calculated using (eqn.8). We can also calculate the non-dimensional domain temperature as follows

\[ T_{\text{non-dim}} = \frac{T - T_2}{T_1 - T_2} = \frac{e^o - e^i}{e^o - e^i} \quad (\text{eqn.} \, 17) \]

The Non-dimensional Temperatures are plotted against non-dimensional \( x \) for different acoustic thicknesses in Fig.5. It is seen that this non-dimensional temperature should match the non-dimensional emissive power from the Heaslet and Warming Problem.

![Non-dim Temperature profiles](image)

Fig.5 Non-dim Temperature profiles

Fig.4 The solution domain and boundary conditions

Silicon Bulk Thermal Conductivity

The Boltzmann solver is used to calculate the bulk thermal conductivity of silicon which is \( \frac{148 \, W}{m \, K} \) for pure silicon. Gray Boltzmann transport equation can be solved in the acoustically thick limit to get an analytical expression for bulk thermal conductivity.

\[ k_{\text{bulk}} = \frac{1}{3} C \nu^2 T_{\text{eff}} \quad (\text{eqn.} \, 17) \]

Specific heat of silicon is \( 1.6 \times 10^6 \, \frac{J}{m^3 K} \) and the group velocity can be taken as \( 6400 \, \frac{m}{s} \). We thus calculate the effective relaxation time to be \( 6.77 \times 10^{-12} \, s \). We use these parameters to solve the Boltzmann transport equation with specular boundary conditions and calculate the thermal conductivity as follows

\[ k = \frac{\text{heat flux} \times L}{\Delta T} \quad (\text{eqn.} \, 18) \]
The result is plotted in Fig. 7 for acoustic thicknesses between 10 and 100. The acoustic thickness is changed by changing the length of the domain.

An error margin exists in the calculation of thermal conductivity because of non-uniform heat flux in the domain for higher acoustic thicknesses. The average thermal conductivity however tends to approach the bulk thermal conductivity for silicon for high acoustic thicknesses. It is important to realize that the thermal conductivity values for low acoustic thicknesses are not realistic because the thermal conductivity definition of \( (eqn.18) \) is applicable only for high acoustic thicknesses.

**EFFECT OF RELAXATION TIME ON THERMAL CONDUCTIVITY**

In order to study the qualitative effect of effective relaxation time on thermal conductivity we plot thermal conductivity calculated using \( (eqn.18) \) versus acoustic thickness in Fig. 8.

For both acoustic thicknesses thermal conductivity increases with the specularity factor. This is easy to understand since diffuse boundaries scatter the propagating phonons in all directions, thus adversely affecting heat transfer. On the other hand specular boundaries do not change the velocity of phonons in the direction of propagation thus having no affect on heat transfer. Also, diffuse boundaries have more affect in the low acoustic thickness case since the domain scattering is comparatively lower and the scattering affect of diffuse boundaries is better able to manifest itself. Fig. 10 shows variation of thermal conductivity with the domain aspect ratio when completely diffuse lateral boundaries are employed. It is seen that with the increased confinement of the domain by diffuse lateral boundaries, the thermal conductivity drastically decreases. The effect of these boundaries is to diffuse the propagating phonons completely so that they are not able to carry heat in a particular direction. As the diffuse boundaries confine the domain their effect is felt on a larger proportion in scattering attributed to lower effective relaxation times. Also, the thermal conductivity becomes constant at low acoustic thicknesses due to absence of scattering.

**SPECULARITY AND CONFINEMENT EFFECTS ON THERMAL CONDUCTIVITY**

The Boltzmann equation is solved again in the domain shown in Fig. 4 but with partially specular and partially diffuse lateral boundaries. This helps us to study the effect of imperfect reflections at the lateral boundaries on heat transfer in the domain. Thermal conductivity for two different acoustic thicknesses is plotted against the specularity factor \( p \) in Fig. 9.

The thermal conductivity decreases with increase in acoustic thickness as expected due to increase
of the phonons in the domain, thus drastically decreasing the thermal conductivity.

CONVERGENCE CHARACTERISTICS

In order to study the convergence characteristics of the Boltzmann solver the number of iterations for convergence were plotted against the acoustic thickness of the problem.

Fig. 11 shows that the convergence is very fast for acoustic thicknesses less than one and increases exponentially with increasing acoustic thickness. At high acoustic thicknesses the coupling between the phonon energy equations for different directions is more and thus the problem becomes increasingly non-linear due to the large solution dependent scattering term, thus slowing the convergence rate.

CLOSURE

The Gray Phonon Boltzmann transport equation was solved using a finite volume technique and an iterative procedure employing the Line-by-line TDMA algorithm. Three types of boundaries, namely thermalizing, specular and diffuse boundaries were modeled. The temperature and heat flux results were compared with published theoretical results for an analogous problem and good agreement was obtained. The Boltzmann solver was used to find the bulk thermal conductivity for silicon with moderate accuracy within the confines of numerical convergence of the problem. The effect of different parameters like effective relaxation time, specularity fraction and confinement of lateral boundaries was studied and physically explained. The convergence problems associated with high acoustic thicknesses was also highlighted.

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References