

Numerical Simulations of Non-equilibrium Energy Transport in Nanostructures using Boltzmann Transport Equation

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ABSTRACT

Heat transfer in nanostructures differ significantly from that in the bulk materials since the characteristic length scales associated with heat carriers, i.e., the mean free path and the wavelength, are comparable to the characteristic length of the nanostructures. Nanostructure materials hold the promise of novel phenomena, properties, and functions in the areas of thermoelectric energy conversion and micro/nano electronic devices. One of the major challenges in micro/nano electronic devices is to study the 'hot spot' generation by accurately modeling the carrier-optical phonon-acoustic phonon interactions. Thermoelectric properties are among the properties that may drastically change at nanoscale. During the last decade, advances have been made in increasing the efficiency of thermoelectric energy conversion using nanostructures. In this paper, the non-equilibrium interaction between carriers and phonons in semiconductor thin films is modeled using the Boltzmann transport model (BTM) for studying the transient characteristics of coupled energy transport. The role of nanocomposites in improving the thermal efficiency of thermoelectric devices is also studied by applying the Boltzmann Transport Equation for modeling thermal transport in nanocomposites. The results of this numerical study can help in identifying efficient nanocomposite configuration for use in thermoelectric devices and in understanding 'hot spots' in micro/nano electronic applications. The future scope of extending the present models to study problems of increasing complexities in nanoscale energy transport is also discussed.

NOMENCLATURE

a	lattice constant
$AlAs$	Aluminium Arsenide
AP	Atomic percentage
AR	Aspect ratio
Bi_2Te_3	Bismuth Telluride
C_C	carrier volumetric heat capacity [J/m^3K]
C_{OP}	optical phonon volumetric heat capacity [J/m^3K]
C_p	phonon volumetric heat capacity [J/m^3K]
D_C	carrier density of states per unit volume [m^{-3}]
D_p	phonon density of states per unit volume [m^{-3}]
E	carrier band energy [J]
E_f	electron Fermi energy [J]
$\vec{F}$	external force vector
f	phonon distribution function
f_C	Fermi-Dirac distribution function

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f_p	Bose-Einstein distribution function
$GaAs$	Gallium Arsenide
Ge	Germanium
$\hbar$	Planck's constant divided by 2π [1.054×10^{-34} Js/Phonon]
I	phonon intensity [$Wm^{-2}sr^{-1}$]
κ_b	Boltzmann constant [J/K]
K_C	carrier thermal conductivity [W/mK]
K_p, k	phonon thermal conductivity [W/mK]
k	phonon wave vector
Kn	Knudsen number [Λ/L]
L	film thickness, nanocomposite dimension [nm]
N_C	carrier number density [m^{-3}]
p	specularity parameter, polarization modes, phonon momentum vector
q	phonon heat flux [W/m^2]
R	reflectivity
$\vec{r}$	position vector
$\vec{s}$	direction vector
S	laser energy source [Wm^{-3}]
Si	Silicon
Sb_2Te_3	Antimony Telluride
T	phonon temperature [K]
T_{AP}	acoustic phonon temperature [K]
T_C	carrier temperature [K]
T_{OP}	optical phonon temperature [K]
T_p	phonon temperature [K]
t	time [s]
t_p	laser pulse duration [s]
u_{AP}	acoustic phonon kinetic energy density per unit solid angle [$Jm^{-3}Sr^{-1}$]
u_C	carrier kinetic energy density per unit solid angle [$Jm^{-3}Sr^{-1}$]
u_{OP}	optical phonon kinetic energy density per unit solid angle [$Jm^{-3}Sr^{-1}$]
$u_{eq(C)}$	carrier equilibrium kinetic energy density [Jm^{-3}]
$u_{eq(p)}$	phonon equilibrium energy density [Jm^{-3}]
$u_{eq(AP)}$	phonon equilibrium kinetic energy density [Jm^{-3}]
v_C	average carrier group velocity [m/s]
v	test function
$\mathbf{v}$	phonon group velocity vector [m/s]
v, v_p	average phonon group velocity [m/s]
x	coordinate
x^*	non-dimensional x-coordinate [x/L]
ZT	non-dimensional thermoelectric figure of merit
α, α_1	single photon absorptivity of Si
β	two-photon absorptivity of Si
γ	Auger recombination coefficient of Si
η	y-directional cosine
Θ	impact ionization coefficient
θ	polar angle [rad]
Λ	phonon mean free path [nm]
λ	phonon wavelength [nm]
μ	x-directional cosine

$\tau, \tau_{(p-p)}$	phonon relaxation time
$\tau_{(c-c)}$	carrier relaxation time
$\tau_{(c-p)}$	carrier-phonon relaxation time
ϕ	laser fluence [Jm^{-2}]
ω	phonon frequency [Hz]
Ω	Solid angle [Sr]
ξ	z-directional cosine

Subscripts

b	boundary
c	phonon scattering
d	diffuse interface
eq	equilibrium
i	interface
p	phonon
x	x-coordinate
y	y-coordinate
z	z-coordinate

1. INTRODUCTION

Over the past decade, the scaling down of feature sizes in microelectronic and thermoelectric devices has renewed interest in understanding the physics underlying thermal transport in small-scale structures. Examples of the thermal management of nanodevices are the heating issues in integrated circuits [1] and in semiconductor lasers [2]. Examples in the manipulation of heat flow and energy conversion include nanostructures for thermoelectric energy conversion [3], thermophotovoltaic power generation [4], and data storage [5]. Since the miniaturization of devices coupled with faster processing speeds leads to an increase in the heat dissipation per unit volume, understanding its effect on device performance is critical. Solid state energy conversion technologies have different thermal requirements. An efficient thermoelectric device, used for the conversion between thermal and electrical energy, requires a high electrical but low thermal conductivity. However, superior thermoelectric materials do not exist naturally in their raw form and multi-material structures must be engineered appropriately for this purpose. The ability to understand, predict and manipulate micro/nanoscale thermal phenomena will inevitably be of great significance in the development of new nanostructured devices.

1.1. Heat transfer in micro/nano electronics

The thermal management of microelectronics has already become a challenging issue. Commercial integrated circuits are currently available with transistors whose smallest lateral feature size is around 65 nm and the thinnest material films are smaller than 2 nm, or only a few atomic layers thick. Such miniaturization has led to tremendous integration levels, with more and more transistors assembled together on a smaller area, together with more functionality. The technology advance is likely to follow the current miniaturization trend as summarized by Moore's law in the coming years [6]. The heat generation and chip temperatures are reaching a level that will prevent the reliable operation of the integrated circuits. The chip-level power densities are currently on the order of 100 W/cm^2 . Generally, it has been assumed that electrons and phonons are under local equilibrium in modeling transport in a solid. However, this equilibrium between the charge carriers can be disrupted in cases of high external electric field. In these cases, the electrons get energized and can be far out of equilibrium with the phonons. This is termed as the 'hot electron effect'. The methods to avoid the hot spots on the chip where higher temperatures occur at localized regions is a relevant topic today for chip and integrated circuit designers.

While much of the attention has been focused on chip level packaging, nanoscale heat transfer effects including the thermal conductivity reduction of thin films and the phonon rarefaction or

ballistic effects may further complicate the problem in the performance and design at the device level. The phonon ballistic effect implies that the device temperature rise can be much higher than the prediction employing the Fourier law. In addition, non equilibrium between optical and acoustic phonons can further increase the local temperature rise [7]. Understanding how the heat is generated and transported at the nanoscale has significant implications for the reliability of nanoelectronic devices. Prediction of hotspot temperatures and positions in MOSFET devices and at metal interconnects is necessary for improving thermal design and reliability of micro/nano electronic devices.

1.2. Nanoscale energy transport in thermoelectric devices

As the name indicates, thermoelectricity involves conversion of energy from thermal to electrical or viceversa using charge and heat transport in solid materials. Thermal energy can be converted into electrical energy using 'Seebeck effect' and electrical current can pump heat at one side and deposit it to the other side based on 'Peltier effect' [8–10]. Thermoelectric energy conversion offers many advantages over other energy conversion technology. Because it is based on solid state devices, it requires no moving parts or fluids. Thus, it is silent, reliable, lightweight and environmentally benign. Despite these advantages, the usages of the device are limited so far due to its low efficiency. The present thermoelectric devices operate at about 10% of Carnot efficiency, whereas the efficiency of a compressor-based refrigerator operates at about 30% of Carnot efficiency [11]. Even so, there are several instances for which thermoelectric energy conversion is the most viable option. For example, the Voyager I and II spacecrafts employed thermoelectric energy conversion as spacecraft power generation system for its long term reliability. If one can increase the efficiency of thermoelectric energy conversion, it would revolutionize energy conversion technology.

The performance of a thermoelectric device is determined by the dimensionless thermoelectric figure of merit, ZT [12], such that

$$ZT = \sigma S^2 T / k \quad (1)$$

where σ is the electrical conductivity, S is the Seebeck coefficient, T is the temperature, and k is the thermal conductivity. Equation (1) is a purely material parameter and does not depend on geometry. Therefore, material selection is a key step toward efficient thermoelectric energy conversion. It turns out that these three materials parameters, S , σ , and k , are interdependent and functions of the free carrier concentration in thermoelectric materials. Thus, it has been found that the best materials for thermoelectricity are heavily doped semiconductors with high atomic mass [13].

In the past, several attempts have been made to improve the value of ZT beyond unity for bulk materials by adding defects and dislocations and by alloying.. However, ZT which was nearly constant for the last five decades, suddenly increased beyond unity around the year 2000 using nanostructures. Venkatasubramanian [14] achieved $ZT = 2.4$ at 300 K with Bi_2Te_3/Sb_2Te_3 superlattices, and Harman et al. [15] achieved $ZT = 1.6$ with $PbSeTe$ -based quantum dot superlattice. These experiments showed that the increase in ZT due to nanostructuring was mainly due to a decrease in thermal conductivity. The thermal conductivity of thermoelectric materials can be reduced using a variety of techniques that contribute to increasing the resistance to heat flow in the lattice. A key thermal issue in thermoelectric energy conversion devices is the presence of non-equilibrium between energy carriers, namely electrons and phonons, at the interfaces between metals and semiconductors. Due to the thermal contact resistance of the interface and disparate electron energy levels, the energy carriers in the metal are out of equilibrium with the semiconductor [16].

In this paper, two important topics are studied with respect to energy transport in nanostructure materials for micro/nano electronic and thermoelectric applications; 1) the role of nanocomposites in improving the thermal efficiency of thermoelectric devices and 2) the interaction between the energy carriers namely electrons/carriers with phonons which lead to a significant non-equilibrium at the semiconductor-metal contacts.

2. MATHEMATICAL MODELS AND FORMULATIONS

In dielectric solid materials, heat is transported by atomic lattice vibrations called phonons. In metals, heat is conducted by free electrons as well as by phonons. Electrons in a metal travel at a velocity typically three orders of magnitude larger than phonons. Thus, compared to the energy carried by phonons, the energy flux carried by electrons is generally much larger. Therefore, in metals, electrons are usually the dominant heat carriers. In case of semiconductors, heat is carried predominantly by phonons, because the free electron density in a normal semiconductor is much smaller than that in a metal.

Nanoscale heat transfer can be divided into several regimes as shown in Figure 1. If the structure is approximately an order of magnitude larger than the mean free path, transport is diffusive. When the structure size is comparable to or smaller than the mean free path, size effects begin to appear and eventually the transport becomes ballistic. We further distinguish the size effects into the classical size effect regime and the quantum size effect regime, depending on the ratio of characteristic length to the carrier wavelength. These regimes are also referred to as the particle and wave regimes or incoherent and coherent transport regimes. In the classical size effect regimes, the phase of the energy carriers can be ignored and their trajectories can be traced, instead. In the quantum size effect regime, the phase information is important and must be considered. Whether the transport is in the classical or quantum size effect regime also depends on whether the interface scattering processes can maintain the phases of the waves depending on the ratio of interface roughness to the carrier wavelength as seen in Figure 1.

2.1. Governing equations

2.1.1. Boltzmann transport equation

The Boltzmann transport equation is appropriate for all the energy carriers - dilute gas molecules, electrons, photons and phonons. It is very general, since macroscopic transport behavior for particles, such as the Fourier Law, Ohm's Law, Newton's shear stress Law, Fick's Law, and the hyperbolic heat equation can all be derived from the Boltzmann equation in the macroscale limit with appropriate

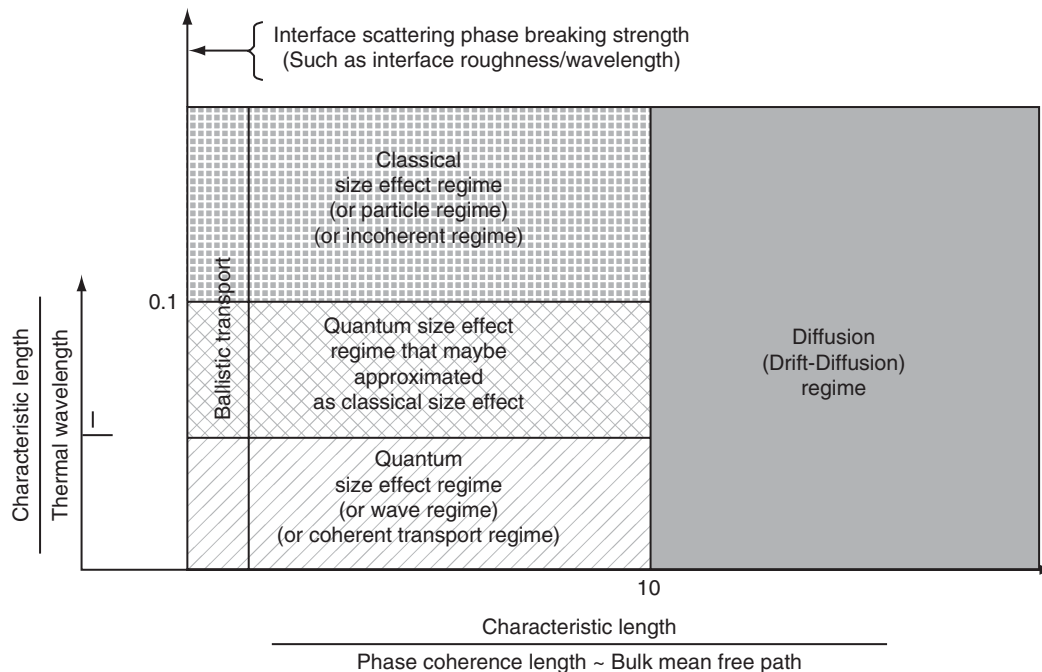


Figure 1. Regimes for treating phonons as either waves or as particles [16].

approximations. From the Boltzmann equation, we can also derive the familiar conservation equations for mass, momentum, energy, and electro-hydrodynamics. In its general form, the BTE can be written as [17, 18]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\vec{r}} f + \vec{F} \cdot \nabla_{\vec{p}} f = \left(\frac{\partial f}{\partial t} \right)_c \quad (2)$$

where f is the statistical distribution function of carriers, which depends on time t , position vector $\vec{r}$, and momentum vector $\vec{p}$. Here $\vec{F}$ is the force applied to the particles. The terms on the left hand side of equation (2) represent the time rate of change of the distribution function, convective transport of the function due to the carrier group velocity, and acceleration due to external forces, respectively. The term on the right hand side of equation (2) represents the scattering term, which restores the system to equilibrium. Quantum mechanical principles are often used to deal with scattering. A general expression of the scattering integral can be formally written, based on the scattering probability and the distribution function. The most basic scattering mechanism is due to the anharmonicity of the lattice potential, which permits phonon-phonon scattering, including normal phonon-phonon scattering and Umklapp phonon-phonon scattering. In nanostructures, phonon-interface scattering dominates the transport at room and higher temperatures. This scattering mechanism is dominant at very low temperature in bulk materials. The evaluation of scattering integrals for phonons is very difficult. Generally, the scattering term can be written as [19]

$$\left(\frac{\partial f}{\partial t} \right)_c = \left(\frac{\partial f}{\partial t} \right)_{e-p} + \left(\frac{\partial f}{\partial t} \right)_{p-p} \quad (3)$$

where $\left(\frac{\partial f}{\partial t} \right)_{e-p}$ is the net phonon generation rate from electron-phonon interaction. $\left(\frac{\partial f}{\partial t} \right)_{p-p}$ denotes the phonon number change due to the phonon-phonon scattering, phonon scattering by lattice defects, and phonon-boundary scattering. Often the relaxation time approximation is used

$$\left(\frac{\partial f}{\partial t} \right)_c = \frac{f_0 - f}{\tau} \quad (4)$$

where f_0 is the Bose-Einstein distribution for phonons at equilibrium temperature T , and τ is the relaxation time as a function of temperature and frequency.

When estimating the effect of several types of scattering centers, each related to a specific relaxation time τ_i , the total time between independent scattering events can be estimated from Mathiessen's rule [19], since the collision term in the Boltzmann equation is proportional to the collision rate and is additive, as shown

$$\frac{1}{\tau} = \sum_i \frac{1}{\tau_i} \quad (5)$$

In analogy to the equation of radiative transfer for photons, the equation of phonon radiative transfer has been derived by Majumdar as [20]

$$\frac{\partial I_\omega}{\partial t} + \mathbf{v} \cdot \nabla_r I_\omega = \frac{I_{\omega,0} - I_\omega}{\tau_\omega} + S_\omega \quad (6)$$

where τ_ω , is the phonon relaxation time, I_ω is the phonon intensity, and S_ω , is due to the phonon generation through the scattering with other carriers, for example, electron-phonon scattering and photon-phonon scattering. The phonon intensity is defined as

$$I_\omega = \nu_\omega \hbar \omega f D(\omega) / 4\pi \quad (7)$$

where $D(\omega)$ is the phonon density of states per unit volume, which should be obtained from the phonon dispersion relation of the specific material.

A rigorous phonon transport simulation should incorporate the frequency dependence of the phonon relaxation time and group velocity, and thus should account for interactions among the dispersive phonons of different frequencies. However, this requires solution of the phonon BTE for many different frequencies. The existing theories for the frequency dependence of the relaxation time contain large uncertainties because they are based on many approximations and rely on the fitting parameters from experimental data. Previous works show that an average relaxation time is a good approximation for thermal conductivity modeling across interfaces [21]. Therefore, we will use a frequency independent phonon relaxation time and phonon group velocity for simplicity, i.e. a phonon gray medium approximation.

For a 3-D system, using the coordinate system shown in Figure 2, the frequency independent BTE can be expressed as [22]

$$\frac{\partial I}{\partial t} + v \left(\mu \frac{\partial I}{\partial x} + \eta \frac{\partial I}{\partial y} + \xi \frac{\partial I}{\partial z} \right) = \frac{I_{eq} - I}{\tau} \quad \text{where } I_{eq} = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 I d\mu d\phi \quad (8)$$

where μ , η and ξ are the x-, y- and z- direction cosines respectively, and v is the average phonon group velocity.

2.1.2. Boltzmann transport model for semiconductors

The carrier-phonon interactions in semiconductor is modeled via the Boltzmann transport model (BTM) consisting of two coupled Boltzmann transport equations (BTEs) one each for carriers namely electron-hole pairs and phonons. The BTEs are formulated in the relaxation time approximation, to describe the energy densities of carriers and phonons denoted by u_C and u_p respectively. The carrier or

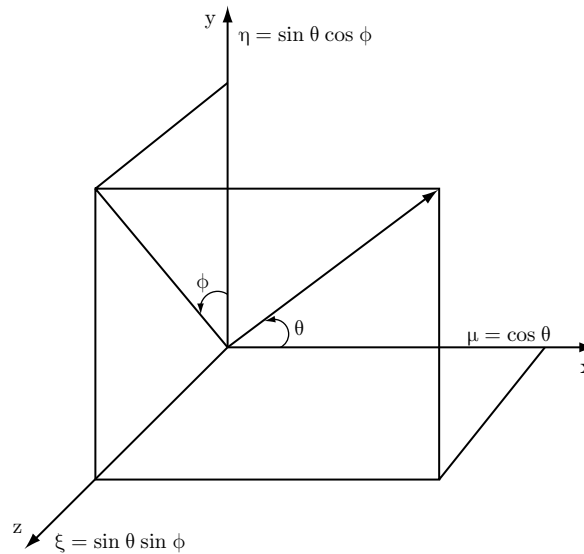


Figure 2. Coordinate system used in the simulations.

phonon energy density is defined as the flux of energy per unit volume and per unit solid angle in the direction $\vec{s}$. The carrier energy density, u_c , is related to its distribution function, f_c

$$u_c(\vec{r}, \vec{s}, t) = \int (E - E_f) f_c(\vec{r}, \vec{s}, t) D_c(E) dE, \quad (9)$$

where $\vec{r}$ denotes the position vector, $(E - E_f)$ is the carrier band energy relative to the Fermi energy and $D_c(E)$ is the carrier density of states per unit volume. The equilibrium distribution of carriers is represented by the Fermi-Dirac distribution [23]. Similarly, the phonon energy density, u_p , is related to its distribution function, f_p [20]

$$u_p(\vec{r}, \vec{s}, t) = \sum \int \hbar \omega f_p(\vec{r}, \vec{s}, t) D_p(\omega) d\omega, \quad (10)$$

where $\hbar$ is the Planck's constant divided by 2π , ω is the phonon frequency, $D_p(\omega)$ is the phonon density of states per unit volume, the integration is over all the phonon frequencies up to the Debye frequency and the summation is over the three phonon polarization modes. The equilibrium distribution of phonons is represented by the Bose-Einstein distribution [19].

When the incident photons have energies greater than the band gap of the semiconductor, electron-hole pairs are formed which act as the heat carriers. The carrier number density of electron-hole pairs, N_c , is determined from the following conservation equation [24]

$$\frac{\partial N_c}{\partial t} = \frac{\alpha_1 S}{h\nu} + \frac{\beta S^2}{2h\nu} - \gamma N_c^3 + \Theta N_c \quad (11)$$

The terms on the right-hand side of equation 11 represent the carrier generation rates from the linear (one-photon) and nonlinear (two-photon) absorption, the Auger recombination, and the impact ionization, respectively.

When the carriers are assumed to transfer their energy directly to the acoustic phonons, the interaction is referred to as the carrier-acoustic phonon interaction. However, the carriers generally interact with the optical phonons directly which then subsequently transfer their energy to the acoustic phonons. This involves a set of equations which consider the energy densities of the carriers, optical phonons, and acoustic phonons and their interactions. The BTM for the case of carrier-optical phonon-acoustic phonon interaction (C-OP-AP) can be expressed as [25]

$$\frac{\partial u_c}{\partial t} + v_c \left(\mu \frac{\partial u_c}{\partial x} \right) = \frac{u_{eq(c)} - u_c}{\tau_{(c-c)}} - \frac{\partial(N_c E_g)}{\partial t} - \frac{C_c(T_c - T_{OP})}{4\pi \tau_{(c-p)}} + \frac{\alpha I(x,t) + \beta I^2(x,t)}{4\pi} \quad (12)$$

$$\frac{\partial u_{OP}}{\partial t} = \frac{C_c(T_c - T_{OP})}{4\pi \tau_{(c-p)}} - \frac{C_{OP}(T_{OP} - T_p)}{4\pi \tau_{(p-p)}} \quad (13)$$

$$\frac{\partial u_{AP}}{\partial t} + v_p \left(\mu \frac{\partial u_{AP}}{\partial x} \right) = \frac{u_{eq(AP)} - u_{AP}}{\tau_{(p-p)}} + \frac{C_{OP}(T_{OP} - T_p)}{4\pi \tau_{(p-p)}} \quad (14)$$

here the subscript *OP* and *AP* denote the optical and acoustic phonons, respectively. The terms on the left-hand side of equation (12) represent the time rate of change of the carrier kinetic energy per unit volume and carrier convective transport, respectively. The terms on the right-hand side of equation (12) represent the carrier-carrier collisions approximated by the relaxation time, time rate of change of the band-gap energy per unit volume, energy loss due to carrier-phonon collisions and the laser source, respectively. The term on the left-hand side of equation (13) represent the time rate of change of the optical phonon kinetic energy per unit volume. The terms on the right-hand side of equation (13) represent the energy gain due to carrier-optical phonon collisions, and the energy loss due to optical-acoustic phonon collisions, respectively. The terms on the left-hand side of equation (14) represent the time rate of change of the acoustic phonon kinetic energy per unit volume and acoustic phonon convective transport, respectively. The terms on the right-hand side of equation (14) represent the phonon-phonon collisions approximated by the relaxation time, and the energy gain due to carrier-phonon collisions, respectively.

The equilibrium energies are given by

$$u_{eq(c)} = \frac{1}{4\pi} \int_{-1}^1 \int_0^{2\pi} u_c d\Omega \quad \text{and} \quad u_{eq(AP)} = \frac{1}{4\pi} \int_{-1}^1 \int_0^{2\pi} u_{AP} d\Omega \quad (15)$$

where μ is the x-direction cosine. The initial energy densities for carriers and phonons are assumed to be constants and are calculated at $T = 300 \text{ K}$. The energy densities obtained from solving the BTEs are used to determine the carrier and phonon temperatures from

$$\int_0^{T_c} C_c dT = u_c(x, \theta) \Delta\Omega \quad \int_0^{T_{OP}} C_{OP} dT = u_{OP}(x, \theta) \Delta\Omega \quad \int_0^{T_{AP}} C_p dT = u_{AP}(x, \theta) \Delta\Omega, \quad (16)$$

where $\Delta\Omega = 4\pi \sin\theta \sin(0.5\Delta\theta)$ is the volume of the ‘finite angle’. The integrals in the equation above are evaluated using trapezoidal rule and the temperatures are obtained iteratively using the bisection method. For the C-OP-AP coupling, the phonon temperature, T_p is defined as,

$$T_p = \frac{C_p T_{AP} + C_{OP} T_{OP}}{C_p + C_{OP}} \quad (17)$$

2.2. Dispersion method for calculating phonon properties

The material properties used in the computation are evaluated using the sine function phonon dispersion model proposed by Chen [21]. This model uses the frequency averaged specific heat and velocity to calculate the phonon mean free path from the relation

$$k = \frac{\Lambda}{3} \sum_p \int_0^{\omega_{mp}} C_{\omega p}(\omega) v_p(\omega) d\omega \quad (18)$$

where ω_{mp} is the maximum allowable frequency corresponding to the polarization p and is related to the Debye temperature. The phonon dispersion relations for nanostructures [26] are obtained along a particular crystal direction and are assumed isotropic in other directions. They are approximated as sine function similar to that of a linear atomic chain.

$$\omega_p = \omega_{mp} \sin(\vec{k}a/2) \quad (19)$$

where a is the equivalent atomic separation of an isotropic medium which can be determined from $a = \pi(6\pi^2/V)^{-\frac{1}{3}}$. Here, V is the volume of the nanostructure molecule. The group velocity and the specific heat for each polarization mode can be expressed as

$$v_p = \frac{\omega_{mp} a}{2} \cos\left(\frac{\vec{k}a}{2}\right) \quad (20)$$

$$C_{\omega p} = \frac{4\hbar^2}{\pi^2 k_b a^3 T^2 \omega_{mp}} \frac{[\sin^{-1}(\omega/\omega_{mp})]^2}{\cos(\vec{k}a/2)} \frac{\omega^2 \exp(\hbar\omega/k_b T)}{[\exp(\hbar\omega/k_b T) - 1]^2}. \quad (21)$$

In the calculation of phonon group velocities, only the acoustic phonon contribution is accounted while neglecting the optical phonon contribution, since, the slopes of the optical phonon dispersion curves are small. The expression for the total specific heat is obtained by integrating the frequency dependant specific heat over the entire frequency range and summing over the acoustic polarization modes

$$C = \sum_p \int_0^{\omega_{mp}} C_{\omega p} d\omega \quad (22)$$

The mean free path can also be calculated from Equation 18. The average group velocity of the phonons are calculated from the expression $k = \frac{1}{3} C v \Lambda$, using the bulk thermal conductivity, mean free path, and the total specific heat calculated from equations (18) and (22).

The Debye model assumes a linear dispersion relationship between the phonon frequency and the wave vector. However, the phonon dispersion model takes into account the non-linear phonon dispersion and therefore gives a more accurate estimate of the material properties.

2.3. Interface treatment

The BTE for the phonon intensity is solved in conjunction with suitable boundary and interface treatment. The treatment of interfaces between the two materials significantly affects the thermal characteristics of the nanostructure. The interfaces between the two materials are modeled as either totally diffuse or totally specular or as a combination of both [27, 28]. For totally diffuse interfaces, the model proposed by Schwartz and Pohl [27] called the Diffuse Mismatch Model (DMM) is used. This model makes an assumption that the phonons emerging from an interface are independent of the phonons incident on the interface. The specular scattering off an interface is modeled using the elastic Acoustic Mismatch Model (AMM) [29].

The intensity of the phonons using the DMM for diffuse interfaces and AMM for specular interfaces are separately calculated and are combined using the interface specularity parameter p defined by Ziman [19] as

$$p = \exp\left(-\frac{16\pi^3 \delta^2}{\lambda^2}\right), \quad (23)$$

where δ is the interface roughness and λ is the characteristic phonon wavelength. Zhang [30] presents this expression with π^2 in the exponent rather than the widely quoted π^3 as shown in equation (23). If

the specularity parameter p is zero, it indicates a totally diffuse or a rough interface and a value of p equal to one indicates a specular or a smooth interface. A real interface is neither truly diffuse nor specular and hence cannot be accurately represented by the two limits. The interfaces can be modeled as diffuse if the interface roughness is greater than the phonon wavelength. Even for values of interface roughness less than the phonon wavelength, equation (23) predicts a high probability for diffuse scattering. Therefore, the value of p is explicitly chosen to combine the diffuse and specular interface treatment models [31].

3. NUMERICAL METHODOLOGY

Modeling the multidimensional heat conduction processes in devices involving multiple length and time scales ranging from nanoscale to macroscale is very challenging. Hence higher order schemes are required to accurately model the disparate length and time scales. The Runge-Kutta Discontinuous Galerkin method [32, 33] is used for the numerical solution of BTE using higher order polynomials for the spatial and angular resolution. The RKDG method incorporates the local conservation property of the finite volume schemes and the higher order accuracy of finite element methods [32]. The DG method has some attractive properties that makes it a good alternative to existing methods for problems described using hyperbolic equations such as those encountered in fluid flows or thermal radiation. These properties include higher-order local approximation using polynomials, ease of parallelization, element-wise conservation and geometric flexibility of conventional finite elements. High resolution temporal discretization is achieved using a four stage Runge-Kutta (RK) time stepping scheme that allows the RKDG method to be numerically stable [33]. In the present computations, for spatial discretization, both piecewise constant and linear Legendre basis functions are employed [34]. All spatial integrations are performed using Gaussian quadrature points and weights. The flux at the interfaces are approximated using a monotone 'upwind' numerical flux scheme.

The numerical solution to the BTE for the nanocomposites are computationally prohibitive on a single processor due to an excessive grid size used for detailed spatial and angular resolution. For the case of nanoparticles, a grid size of $128 \times 128 \times 128 \times 30 \times 20$ which includes three spatial and two angular dimensions is used. The CPU time required to solve the 3-D BTE on a single processor would incur approximately 3 months for the former case and approximately 20 days for the latter case. Therefore, a parallel algorithm has been developed to speed-up the computations. The 3-D BTE solver is parallelized in the x- and y- directions using Message Passing Interface (MPI) communication routines [35]. In this algorithm the computational domain is split up into a number of subdomains equal to the number of processors assigned to perform the simulation. The ratio between the communication time and the total computation time directly affects the efficiency of the parallel code. By increasing the number of processors, the subdomain size decreases. The scalability of the parallel code is measured by performing simulations using a fixed subdomain size on an increasing number of processors. The scalability is defined as the ratio of time taken for the code to run on two processors to the time taken to run on N processors. Figures 3(a) and 3(b) show the parallel efficiency study conducted using the Dell Linux cluster at Center for computational Research (CCR) at the University at Buffalo and the IBM Linux Cluster at NCSA's super computing center. Two different grids of sizes $64 \times 64 \times 64 \times 30 \times 20$ and $128 \times 128 \times 128 \times 30 \times 20$ are tested for the case of energy transport in nanoparticles. Figures 3(a) shows the CPU time taken per time step for the different grid sizes when run on both the CCR and NCSA clusters. The CPU time taken for the larger grid size at both the CCR and NCSA clusters show similar values with increasing number of processors. For the grid size of $128 \times 128 \times 128 \times 30 \times 20$, the parallel computations incur a CPU time per time step of 12 seconds utilizing 64 processors. The scalability study shown in Figure 3(b) indicates a near-linear scale-up from 2 to 64 processors for the smaller grid size. The code for the larger grid size also demonstrates a good scalability beyond 32 processors.

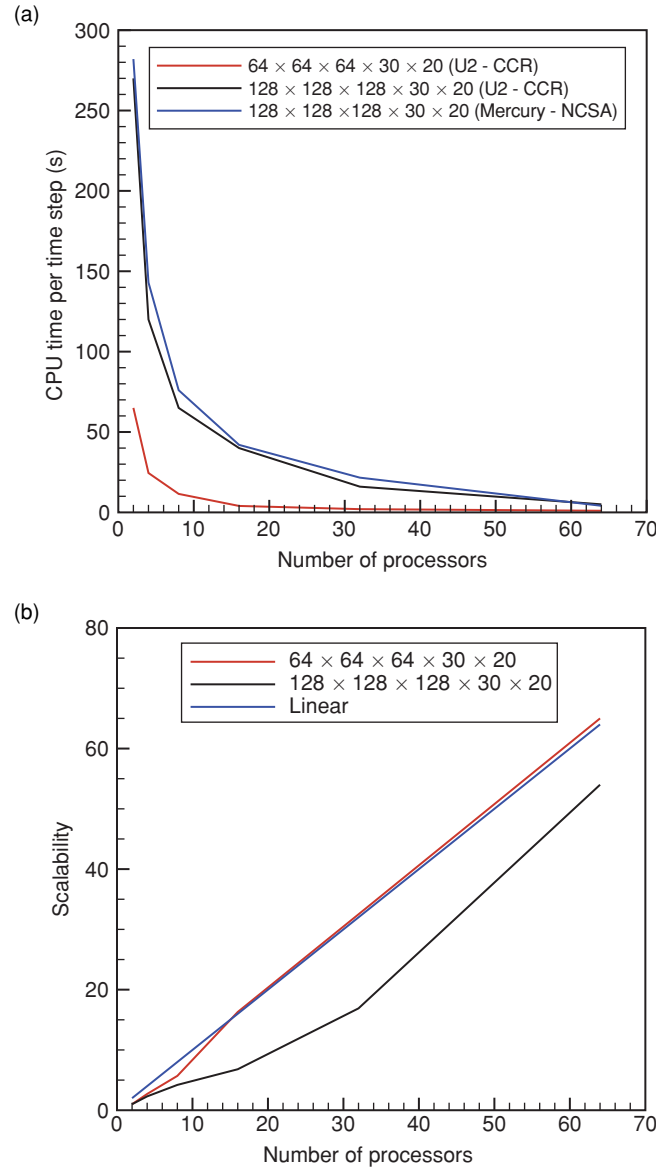


Figure 3. (a) CPU times and (b) Scalability of the parallel code.

4. RESULTS AND DISCUSSION

The Boltzmann Transport equation (BTE) is validated for steady state heat transport across the Bi_2Te_3 - Sb_2Te_3 superlattice. The superlattice consists of periodically repeating stacks of Bi_2Te_3 on Sb_2Te_3 layers with heat transport across the layers. It is useful in studying the role of interface in the reduction of thermal conductivity. Figure 4 shows the effective thermal conductivity, k , plotted as a function of the superlattice period thickness. This figure shows a reduction in the thermal conductivity with decreasing period thickness of the superlattice. Here the period thickness denotes the combined thicknesses of the two materials. This reduction is caused by the thermal boundary resistance to phonon transport, when the mean free path (MFP) of the phonons is greater than the half period thickness [27, 36]. A study of varying the specularity parameter, p , is conducted to understand the effect of interface roughness on thermal conductivity of the superlattice. This study

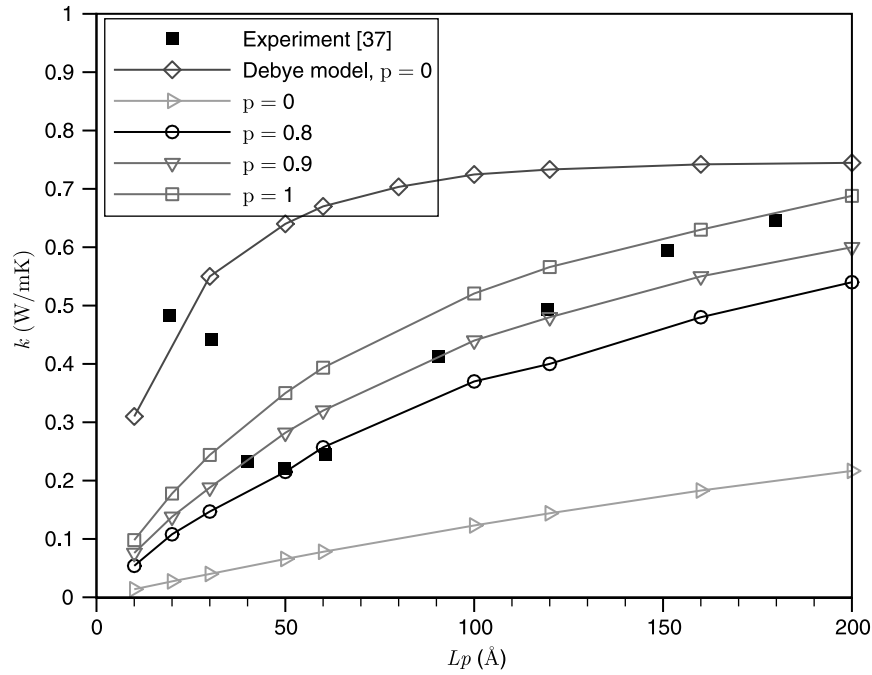


Figure 4. Variation of thermal conductivity with period thickness for $\text{Bi}_2\text{Te}_3\text{-Sb}_2\text{Te}_3$ superlattice.

shows an increase in the thermal conductivity with increasing values of p . For diffuse interface, the phonon scattering occurs in all directions. Consequently, this causes a reduction in the heat flow and hence a smaller value of k is obtained. Whereas, in the case of $p = 1$, most of the scattering occurs along the heat flow direction resulting in higher value of k .

The experimental data of Venkatasubramanian [37] is also shown in Figure 4. These data show a similar decrease in thermal conductivity with reducing period thickness up to 50 Å. For thickness values less than 50 Å, the thermal conductivity increases and approaches the bulk value. Although the reasons for this behavior are not clear, some explanations pointing to the wave nature of phonons have been offered in the literature. Although, the experimental data is scattered within the band of 0.8–1, the predicted thermal conductivity for $p = 0.9$ gives the smallest root mean square (RMS) error of 15% when compared to data while, $p = 0$ shows the maximum error of 76%. This indicates that the actual interface scattering can neither be modeled as totally diffuse nor totally specular. The Debye model predicts thermal conductivity values which are not in accordance with the experimental data. This is due to MFP of the phonons calculated from the Debye model being smaller than the superlattice thickness, even for the period thickness of 50 Å. Consequently, the result with Debye model is closer to the macroscopic regime and cannot capture the ballistic effects observed in the experiment.

4.1. Heat transport in nanocomposites

Nanocomposites may realize thermal conductivity reduction and provide a pathway to scale-up the nanoscale effects observed in superlattices to actual thermoelectric devices. There are not many theoretical and computational studies on the thermal conductivity of nanocomposites, despite their importance for practical applications such as for thermoelectric applications. In this section, the deterministic solution of the phonon Boltzmann equation is used to study the thermal conductivity of 3-D nanocomposites where nanoparticles are periodically aligned in a host matrix. Results of this study can be used to direct the development of high efficiency thermoelectric materials and thermal interface materials for micro/nano electronic applications with high thermal conductivity.

4.1.1. Problem definition

The schematic of the nanoparticle composite chosen for the present simulations and the 3-D coordinate system used in the simulations are shown in Figure 5. The nanoparticle composite consists of either cubic or non-cubic nanoparticles dispersed in a cubic host, as shown in Figure 5 (a). Although, in practice, these nanoparticles may be randomly distributed in the host, the uniform distribution considered here offers computational simplicity. The materials considered for the host are Bismuth Telluride (Bi_2Te_3), Germanium (Ge), and Gallium Arsenide ($GaAs$) and the corresponding materials for particles are Antimony Telluride (Sb_2Te_3), Silicon (Si), and Aluminum Arsenide ($AlAs$) respectively. The nanoparticles are assumed to be uniformly distributed inside the host material. The heat is applied along the x- and z- directions. The 3-D unit cell as shown in Figure 5(b) is used to simulate the effect of a single particle and the surrounding host material within the cell.

The BTE for the phonon intensity in 3-D given by equation (8) is solved in conjunction with suitable boundary and interface treatments. The material properties used in the computation are evaluated using the phonon sine function dispersion model proposed by Chen [38]. Table 1 summarizes the properties of Ge , Si , $GaAs$, $AlAs$, Bi_2Te_3 and Sb_2Te_3 calculated using the dispersion model at 300 K.

In the present case, the interface is treated as totally diffuse and the Diffuse Mismatch Model (DMM) [27] is used. The top and the bottom boundaries of the unit cell are treated as adiabatic surfaces and the remaining boundaries are modeled as periodic, to maintain continuity of heat flow. [31]. The adiabatic condition is modeled as a specularly reflecting boundary on which the following condition for intensity is imposed:

$$I(\vec{r}_b, \vec{s}, t) = I(\vec{r}_b, \vec{s}_r, t) \quad (24)$$

where $\vec{s}_r = \vec{s} - 2(\vec{s} \cdot \vec{n})\vec{n}$, $\vec{n}$ is the outward normal vector, and $\vec{r}_b$ denotes the spatial coordinates of the boundary.

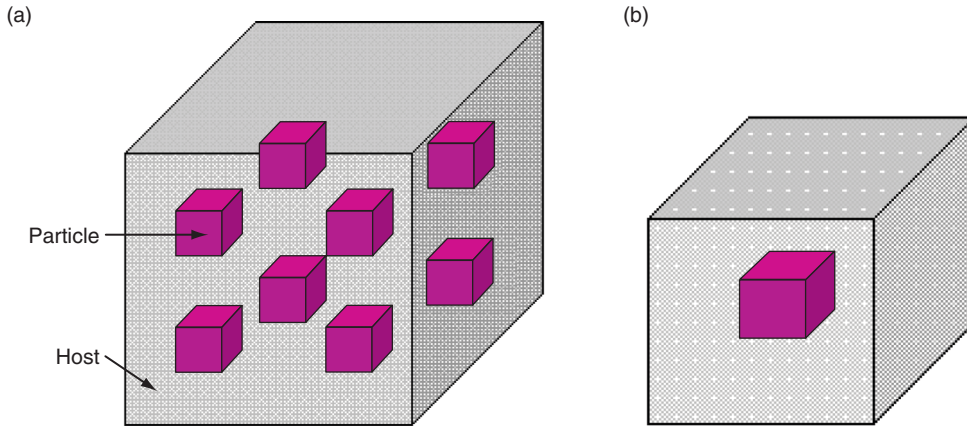


Figure 5. Schematic of (a) Nanoparticle composite and (b) Unit cell.

Table 1. Material properties calculated using phonon sine function dispersion model.

Material	k (W/mK)	$C \times 10^6$ (J/m ³ K)	v (m/s)	Λ (Å)
Ge	60	0.87	1042	1986
Si	145.6	0.93	1804	2604
GaAs	43.6	0.88	1024	1453
AlAs	86.4	0.88	1246	2364
Bi_2Te_3	1.1	0.5	212	310
Sb_2Te_3	0.9	0.53	200	254

The parameters that have been varied to study their effect on the thermal characteristics of the nanoparticle composite are the particle size, atomic percentage (AP), and the particle aspect ratio (AR). The atomic percentage of the nanoparticle is related to the volumetric percentage, VP , and the lattice constant, a , as [31]

$$AP = \frac{VP}{\left[VP + (1 - VP) \frac{a_p}{a_h} \right]} \quad (25)$$

For the cubic nanoparticle composite, $VP = \frac{L_p^3}{L_h^3}$, where L_p and L_h are the lengths of the particle and host respectively. Aspect ratio, AR , is defined as the ratio of nanoparticle length in the z-direction to its length in the x-direction, L_z/L_x .

The phonon intensity obtained from solving the BTE is then used to determine the heat flux, temperature distribution, and thermal conductivities. At nanoscales, the temperature, as such, has no physical meaning except that it is an indicator of the local energy density of the system. The effective temperature is obtained from phonon intensity as

$$T(x, y, z) = \frac{1}{C_h v_h} \sum_{N_\theta} \sum_{N_\phi} I(x, y, z, \theta, \phi) w_\theta w_\phi \quad (26)$$

where w_θ and w_ϕ are the weights associated with the polar and azimuthal directions respectively. The heat fluxes in the x and z directions namely q_x and q_z are related to the intensity through the relations

$$q_x(x, y, z) = \sum_{N_\theta} \sum_{N_\phi} I(x, y, z, \theta, \phi) \mu w_\theta w_\phi \quad (27)$$

$$q_z(x, y, z) = \sum_{N_\theta} \sum_{N_\phi} I(x, y, z, \theta, \phi) \xi w_\theta w_\phi \quad (28)$$

For the non-cubic nanoparticle composite, the effective thermal conductivities in the x-direction, k_x , and in the z-direction, k_z , can be defined as

$$k_x = \frac{Q_x L_x}{L_y L_z (\bar{T}(x=0) - \bar{T}(x=L_h))}; k_z = \frac{Q_z L_z}{L_x L_y (\bar{T}(z=0) - \bar{T}(z=L_h))} \quad (29)$$

where Q_x and Q_z are the heat flow in the x- and z- directions respectively. $\bar{T}$ is the area averaged temperature at the boundary. For the cubic nanoparticle composite, $k = k_x = k_y$ due to symmetries in geometry and heat flow in all three coordinate directions.

4.1.2. Temperature contours

The steady state heat transport simulations are performed for the cubic Sb_2Te_3 nanoparticle suspended in Bi_2Te_3 host material. The nature of phonon transport is characterized by a non-dimensional ratio of phonon mean free path to the particle size, called the Knudsen number, Kn . $Kn \gg 1$ indicates ballistic limit and $Kn \ll 1$ indicates Fourier limit. Figure 6(a) shows $T - T_{ref}$ temperature contours for a Kn of 10 with heat transport in both x- and z- directions. The reference temperature $T_{ref} = 300$ K.

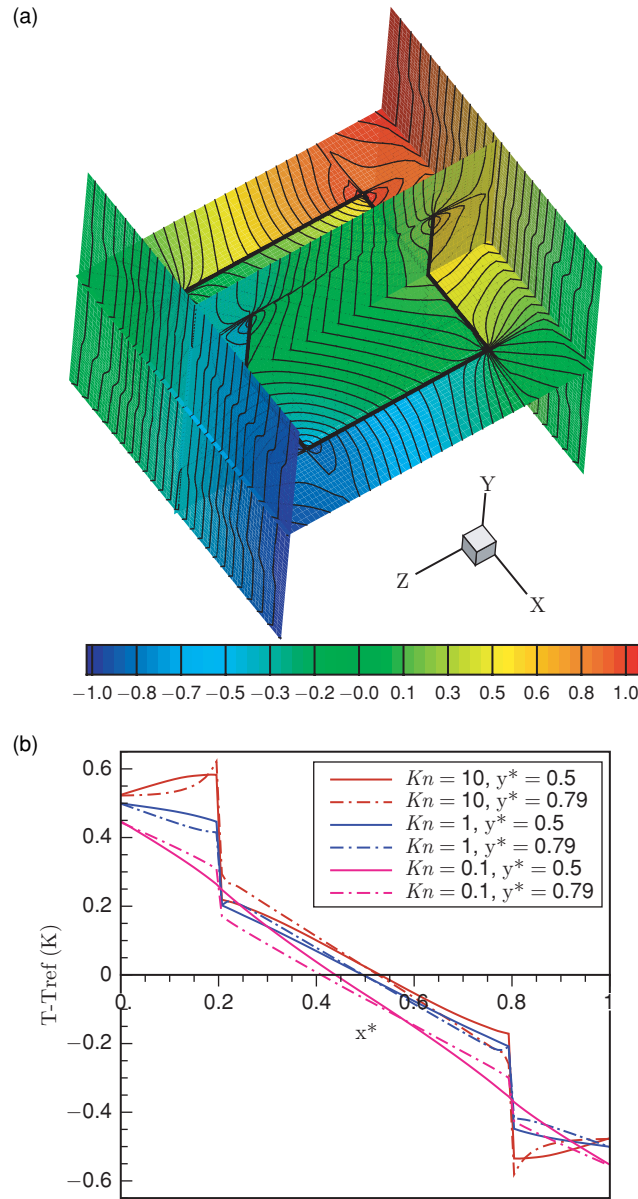


Figure 6. (a) Temperature contours for Bi_2Te_3 - Sb_2Te_3 nanoparticle composite for $\text{AP} = 0.2$ and $L_{\text{Sb}_2\text{Te}_3} = 25.4 \text{ \AA}$ and (b) Temperature profiles ($T - T_{\text{ref}}$) for $\text{AP} = 0.2$.

The same temperature difference is applied in both directions leading to a heat flux ratio q_x/q_z of 1. The temperature contours indicate significant non-linearity in the temperature distribution both inside the particle as well as in the host due to significant phonon scattering at the interfaces between the two materials. The contours are clustered near the interfaces where the interface scattering dominates the interior scattering of phonons. To better understand the effects of scattering from the particle interfaces, the temperature profiles are shown at two different y -locations as seen in Figure 6(b). In the x - y plane, these are at midway, $y^* = 0.5$, and through the top interface at $y^* = 0.79$. The temperature jumps occurring at the interface between the host and the particle can be attributed to interface thermal resistance which has also been observed for lower dimensional nanostructure configurations such as the superlattice and nanowire composites [31, 39]. In order to compare the effect of Kn on the temperature, its profile for the ballistic case of $Kn = 10$ is compared with the transitional ($Kn = 1$) and Fourier

($Kn = 0.1$) cases. For the case of $Kn = 10$, the left interface has a higher temperature, and the right interface has a lower temperature than the boundary temperatures resulting in a change in the sign of temperature gradient along the x-direction. Similar results were obtained by Yang and Chen [39] and by Pattamatta and Madnia [31] in the ballistic limit for $Ge-Si$ and $Bi_2Te_3-Sb_2Te_3$ nanowire composites, respectively. However, this is not observed for the lower Kn number cases where ballistic effects are less pronounced. The temperature profiles in the y-z plane corresponding to heat flow in the z-direction also show similar trend as in the x-direction due to the cubic nature of the nanoparticle and due to uniform heat fluxes in both of these directions.

4.1.3. Thermal conductivity and figure of merit

The variation of effective thermal conductivity, k , of the cubic $Bi_2Te_3-Sb_2Te_3$ nanoparticle composite with the particle size, for atomic percentages of 0.2 and 0.8 is shown in Figure 7(a). As a reference, the thermal conductivities for $Bi_2Te_3-Sb_2Te_3$ superlattice and 2-D $Bi_2Te_3-Sb_2Te_3$

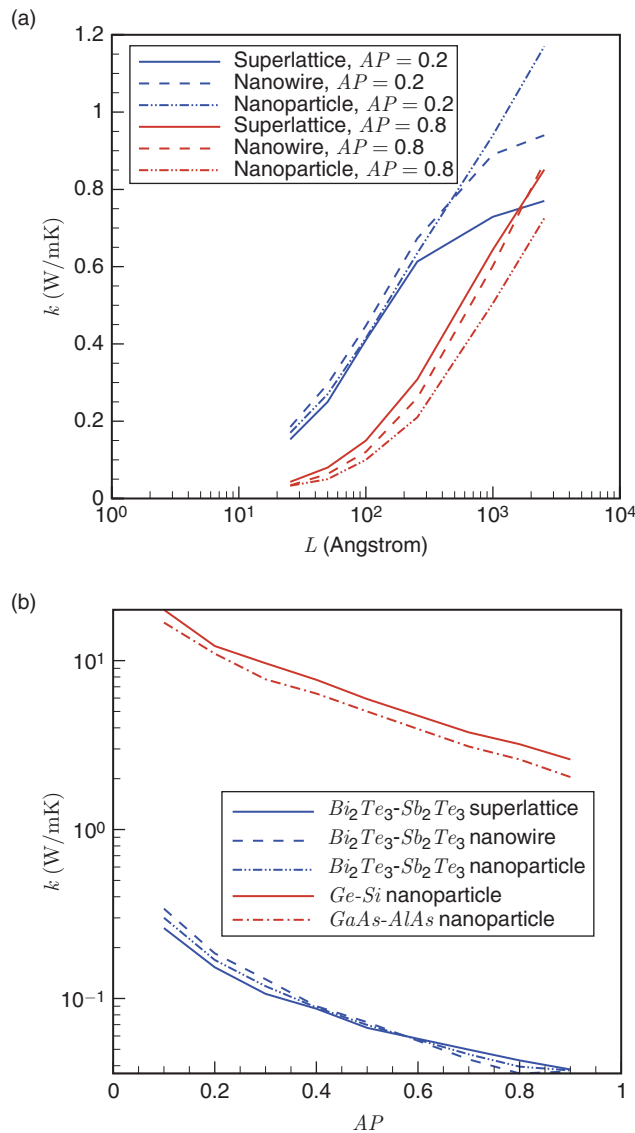


Figure 7. (a) 'Size effect' on thermal conductivity of $Bi_2Te_3-Sb_2Te_3$ nanocomposites. (b) Effect of atomic percentage on thermal conductivity of nanostructures for $Kn = 10$.

nanowire are also shown on the this figure. The thermal conductivity decreases with decreasing particle size. This is attributed to the increase in phonon scattering at the interfaces of the nanoparticle due to ballistic effects, with decreasing particle size [39]. The dependence of thermal conductivity on particle size is called the ‘classical size effect’. For $AP = 0.2$, the values of thermal conductivity of the cubic nanoparticle composite is close to that of 1-D superlattice and 2-D nanowire composites. For larger sizes, the thermal conductivities of the nanoparticle, nanowire and superlattice composites approach their respective bulk values, the bulk value of nanoparticle composite being higher than the nanowire and superlattice composites. However, for the case of $AP = 0.8$, for particle sizes above 100 Å, the thermal conductivity of the nanoparticle composite is lower than the nanowire and superlattice composites. For particle sizes less than 25 Å, where the phonon wavelength becomes comparable to the dimension of the nanoparticle, wave effects may need to be considered in predicting the value of k . Figure 7(a) also shows that for a given wire size, the thermal conductivity corresponding to $AP = 0.8$ is lower than that of $AP = 0.2$, due to an increase in ballistic effects in the host for $AP = 0.8$. Figure 7(b) shows the effect of atomic percentage on the thermal conductivity of $Bi_2Te_3-Sb_2Te_3$, $Ge-Si$, and $GaAs-AlAs$ nanocomposites. The atomic percentage is varied from 0.1 to 0.9 keeping the particle Kn fixed at 10. For a given particle size, increasing the atomic percentage results in a decrease in the size of the host. This results in higher phonon interface scattering and hence a decrease of thermal conductivity. The thermal conductivity values for 3-D $Bi_2Te_3-Sb_2Te_3$ nanoparticle composite is similar to the superlattice and nanowire composites. The $Ge-Si$ and $GaAs-AlAs$ nanoparticle composites show similar atomic percentage effects but their thermal conductivities are approximately two orders of magnitude higher than that of $Bi_2Te_3-Sb_2Te_3$.

Table 2 shows the comparison of thermoelectric properties and ZT for $Bi_2Te_3-Sb_2Te_3$ Superlattice and nanocomposite. The computed values of k corresponding to $AP = 0.5$ and $p = 0.9$ are 0.26 and 0.28 for the nanocomposite and superlattice respectively. The value of $p = 0.9$ is chosen since the best match between the simulation and experiment for the superlattice is obtained for this value. The values of k for the nanocomposite vary between 0.034–0.74, depending on the atomic percentage and interface treatment. The electron properties such as the Seebeck coefficient and electrical conductivity may actually vary for the nanocomposite configuration. For the sake of comparison, we use the power factor of superlattice [14] to estimate the ZT for the nanocomposite. Thus, assuming a power factor, $S^2\sigma$, equal to the superlattice power factor, values of ZT in the range of 0.71–15.5 is obtained for the nanocomposite. This highlights the importance of using $Bi_2Te_3-Sb_2Te_3$ nanostructures for efficient thermoelectric applications.

4.1.4. Comparison of BTE with Fourier results

In order to highlight the limitations of the Fourier model when applied to heat transport in nanoparticle composites, comparison is made between the BTE and Fourier solution and shown in Figure 8. Figures 8(a) and (c) show the relative percentage differences between the BTE and Fourier temperature prediction for the $Bi_2Te_3-Sb_2Te_3$ non-cubic nanoparticle composite plotted in the x-y and x-z planes respectively. The relative percentage difference is expressed as $(T_{BTE} - T_{Fourier}) * 100 / T_{BTE}$. The

Table 2. Thermoelectric properties of $Bi_2Te_3-Sb_2Te_3$ superlattice and nanocomposite.

Material	Method	AP	P	k (W/mK)	$S^2\sigma$ (10^{-3} W/mK ²)	ZT
$Bi_2Te_3-Sb_2Te_3$ SL	Experiment [14]	0.5	–	0.22	1.76	2.4
$Bi_2Te_3-Sb_2Te_3$ SL	Simulation	0.5	0.9	0.28	1.76	1.89
$Bi_2Te_3-Sb_2Te_3$ NC	Simulation	0.5	0.9	0.26	1.76	2.03
$Bi_2Te_3-Sb_2Te_3$ NC	Simulation	0.1–0.9	0–1	0.034–0.74	1.76	0.71–15.5

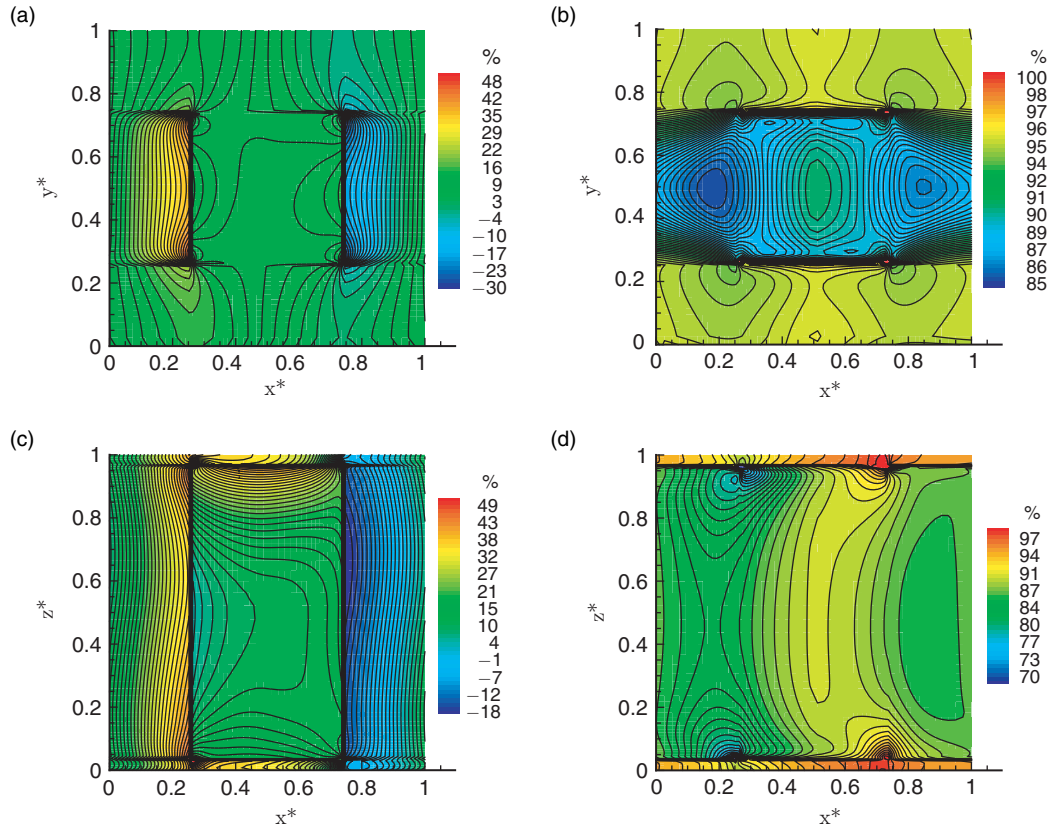


Figure 8. Percentage difference between BTE and Fourier simulations as observed in (a), (c) temperature contours and (b), (d) heat flux contours for a non-cubic $Bi_2Te_3-Sb_2Te_3$ nanoparticle composite. $Kn = 10$, $AP = 0.2$, and $AR = 2$.

positive values indicate under-prediction by the Fourier model. The regions near the interface of the two materials, where the maxima and minima in the temperatures occur, show the maximum differences between the two models. The Fourier model under-predicts regions of maximum temperature by as much as 50% and over-predicts the regions of minimum temperature by 30%. This is consistent with the results of nanoscale Silicon-on-Insulator (SOI) in which the regions of peak phonon temperatures or ‘hot spots’ are significantly underestimated in the Fourier solution [40]. Figures 8(b) and (d) show the percentage difference in x-direction heat fluxes between the BTE and Fourier models for the two planes. The Fourier model underestimates the heat flux throughout the nanocomposite by as much as 100%. In the x-y plane, the percentage difference varies between 85 to 100 percent, whereas, in the x-z plane, it varies between 70 to 100 percent.

4.2. Carrier-phonon Non-equilibrium in Semiconductor thin films

In this section, we investigate carrier-phonon non-equilibrium created due to ultrashort-pulsed laser irradiation on thin silicon films. The non-equilibrium between energy carriers is modeled via numerical solution of the BTM for carriers and phonons which is applicable over a wide range of length and time scales. The carrier interactions with both optical and acoustic phonons are considered. The model is used to study laser heating of nanometer size silicon films, by varying parameters such as the laser fluence and pulse duration for a fixed film size. The results of this study can help in addressing the non-equilibrium at the semiconductor-metal contacts of thermoelectric devices and in modeling ‘hot-spots’ in microelectronic devices.

4.2.1. Problem description

The carrier-phonon interactions are studied by applying a laser beam with a wide range of pulse duration and fluence to a Silicon (Si) film with thicknesses in the range of nano to micrometers. The laser beam diameter is much larger than the optical and carrier penetration depths and hence a one-dimensional model can describe the physical problem [41]. The laser intensity is given as [24],

$$I(x,t) = \frac{2\sqrt{\ln 2} \phi (1-R)}{\sqrt{\pi} t_p} \exp\left(-\int_0^x \alpha dz\right) \exp(-4\ln 2 ((t-2t_p)/t_p)^2) \quad (30)$$

where ϕ is the fluence carried by the laser pulse, R is the reflectivity, t_p is the laser pulse duration defined as full width at half maximum of the laser pulse shape, α is the absorptivity of Si, x is the depth measured from the front surface. The laser beam is Gaussian in both time and space. From equation (30), the peak of the laser intensity occurs at time $t = 2t_p$. The laser wavelength, λ , chosen for the present study is 550 nm.

The carrier-phonon interactions in semiconductor is modeled via the Boltzmann transport model (BTM) consisting of three coupled Boltzmann transport equations (BTEs) one for carriers namely electron-hole pairs and one each for the acoustic and optical phonons, respectively. The carrier-optical phonon-acoustic phonon interaction (C-OP-AP) given by equations (12–14), are considered. The solution to the BTM requires knowledge of carrier and phonon relaxation times, group velocities, thermal conductivities and heat capacities which are listed in Table 3. The physical properties of

Table 3. Physical properties of Si.

Property	Value	Ref.
C_c (J/m ³ K)	$3N_c k_B$	[42]
C_p (J/m ³ K)	Table 2	[42]
C_{OP} (J/m ³ K)	7.15×10^5	[26]
k_c (W/mK)	$-0.556 + 7.13 \times 10^{-3} T_c$	[42]
k_p (W/mK)	Table 2	[26]
v_c (m/s)	$\sqrt{(3k_b T_c)/(2.3 \times 10^{-31})}$	—
v_p (m/s)	Table 2	[26, 43]
τ_{c-c} (S)	$3K_c/(C_c v_c^2)$	—
τ_{c-p} (s)	$\tau_0[1 + (N_c/N_{cr})^2]$ $\tau_0 = 0.5 \times 10^{-12}$ $N_{cr} = 2 \times 10^{27}$	[42, 44]
τ_{p-p} (s)	$3K_p/(C_p v_p^2)$	—
E_g (eV)	$1.167 - 0.0258[T_p/300] - 0.0198 [T_p/300]^2$	[45]
α (1/m)	$\alpha = \alpha_1 + \sigma_{fc} N_c$ $E' = (h\nu) + 1.1214 - E_g$ $\alpha_1 = 250000 * \exp(2.48 * (E' - 1.79))$ $\sigma_{fc} = 5.1 \times 10^{-23} [1.17/(h\nu)]^2 [T_p/300]$	[45]
β (m/W)	2.0×10^{-11}	[44]
Θ (1/s)	$3.6 \times 10^{10} \exp(-1.5 E_g / k_b T_c)$	[44]
γ (m ⁶ /s)	3.8×10^{-43}	[42]
R	0.32	[44]

Table 4. Phonon properties.

T (K)	K_p (W/mK)	$C_p \times 10^6$ (J/m ³ K)	v_p (m/s)
300	154.80	0.96	1740
400	99.90	0.9950	1690
500	70.10	1.01	1670
600	60.30	1.02	1660
700	50	1.02	1650
800	41.70	1.02	1640
900	36	1.02	1630
1000	30	1.02	1620

Silicon used in the present simulations are listed in Table 4. The phonon specific heat and group velocity are calculated as a function of temperature using the phonon sine function dispersion model of Chen [21, 31]. Linear interpolation is used to calculate the properties between any two temperatures given in Table 4. During the very short duration of laser heating, heat losses from the front and back surfaces of the semiconductor are found to be negligible and hence treated as adiabatic. These surfaces are modeled as specularly reflecting boundaries on which the following conditions on carrier and phonon thermal intensities are imposed:

$$u_c(0, \mu, t) = u_c(0, -\mu, t) \quad ; \quad u_c(L, -\mu, t) = u_c(L, \mu, t) \quad (31)$$

$$u_{AP}(0, \mu, t) = u_{AP}(0, -\mu, t) \quad ; \quad u_{AP}(L, -\mu, t) = u_{AP}(L, \mu, t) \quad (32)$$

where μ is the x-direction cosine.

4.2.2. Comparison of BTM with two-temperature model

The results of the BTM with C-OP-AP coupling is compared with the results of the two-temperature models of Lee et al [46] and Chen et al [47] in Figures 9(a) and 9(b), respectively. Figure 9(a) shows the time evolution of the carrier number density and the carrier temperature at the front surface for a Si film thickness $L = 2 \mu m$, laser pulse duration $t_p = 75 fs$ and laser fluence $\phi = 38.2 J/m^2$. The physics of carrier-phonon non-equilibrium for this case cannot be accurately captured using the classical two-temperature model since the laser pulse duration is much smaller than the carrier-phonon relaxation time of 500 fs. It is observed from Figure 9(a) that the peak carrier number density obtained using the BTM is approximately an order of magnitude smaller than the peak number density obtained from the two-temperature model by Lee et al [46]. The value of peak carrier temperature obtained by Lee et al [46] is approximately 35% higher than that of the BTM. This may be due to the excessive diffusion present in the two-temperature model which leads to over-prediction of peak carrier temperature. This excessive diffusion is also observed with the two-temperature models when applied to the case of laser heating of metal films [48]. The BTM model, due to its hyperbolic nature can model the transport of carriers and phonons more realistically without excessive diffusion. Figure 9(b) shows the comparison of the carrier and phonon temperatures between the BTM and the computations of Chen et al [47]. The parameters for this case correspond to a Si film thickness $L = 20 \mu m$, laser pulse duration $t_p = 500 fs$ and laser fluence $\phi = 1500 J/m^2$. The two-temperature model used in the computations of Chen et al. [47] are similar to that used by van Driel [44]. From Figure 9(b), it is observed that the carrier temperature has a double peak which is predicted by both the BTM and the two-temperature models. The first peak in carrier temperature is attained due to the laser excitation of carriers while the second peak is attributed to the Auger recombination process. In Silicon film, band-to-band Auger recombination occurs simultaneously with the collision between two like carriers. The energy released by the recombination process is transferred during the collision to the surviving carrier. Subsequently,

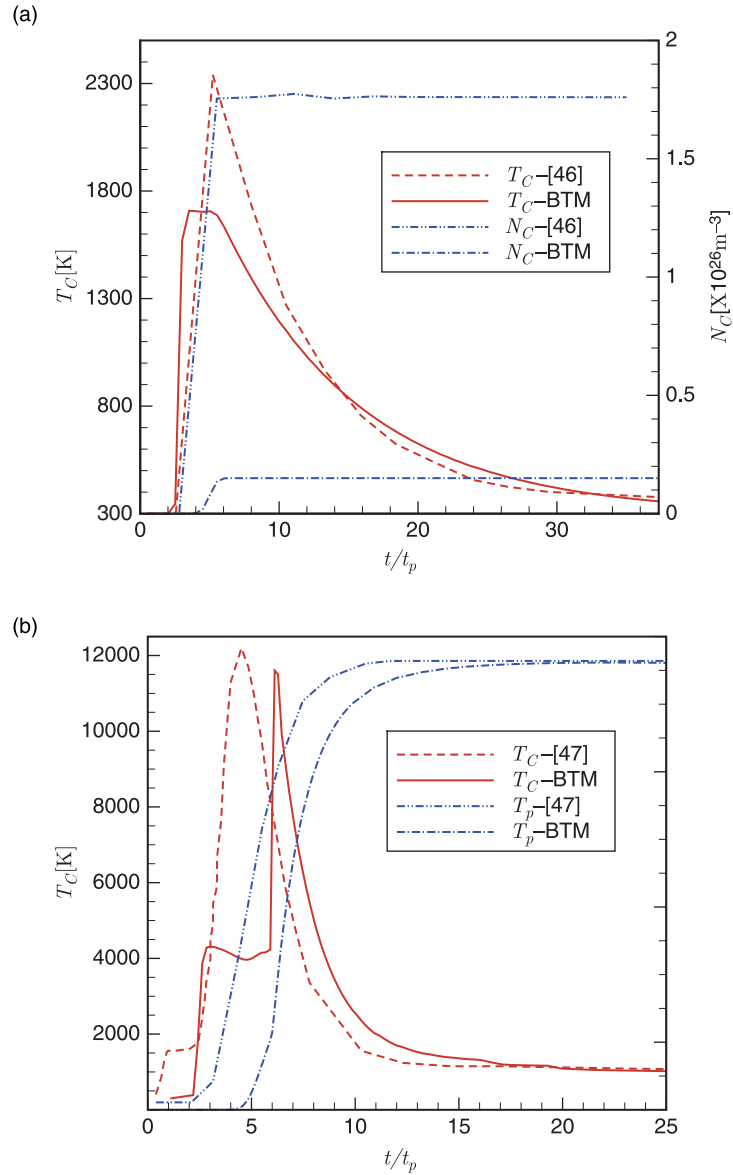


Figure 9. (a) Carrier temperature and number density profiles at the front surface of a Si film for $L = 2 \mu\text{m}$, $t_p = 75 \text{ fs}$ and $\phi = 38.2 \text{ J/m}^2$ and (b) Carrier and phonon temperature profiles at the front surface of a Si film for $L = 20 \mu\text{m}$, $t_p = 500 \text{ fs}$ and $\phi = 1500 \text{ J/m}^2$.

this highly energetic carrier “thermalizes” and loses energy in small steps through collisions with the phonons [49]. Consequently, this causes the phonon temperature to increase till an equilibrium is attained between the carriers and phonon temperatures. Figure 9(b) shows that for this case, the time evolution of T_c and T_p predicted by BTM and Chen et al [47] differ from each other. The first peak in T_c , predicted by the BTM, is higher than that of Chen et al’s [47] Model. The location of peak carrier temperature predicted by the models are different from each other but the value of second peak in carrier temperature predicted by both models are close to each other. The equilibrium temperature predicted by the BTM is in good agreement with that of the Chen et al [47] as seen in Figure 9(b).

Figure 9(b) shows the comparison of the carrier and phonon temperatures between the BTM and the previous computations of Chen et al [47]. The parameters for this case correspond to a Si film

Table 5. Summary of parameters.

Category	L (nm)	t_p (ps)	ϕ (J/m ²)
1	28	0.05–10	500
2	28	0.075	10–3000

thickness, $L = 20 \mu m$, laser pulse width, $t_p = 500 fs$ and laser fluence, $\phi = 1500 J/m^2$. The two-temperature model used in the computations of Chen et al [47] are similar to that used by van Driel [44] which take in to account the work done due to the energy current generated due to the large temperature gradients. Figure 9(b) shows that for this case, the peak carrier temperature profiles predicted by both the models are close to each other. However, the BTM predicts a larger value in the first peak of the carrier temperature. The location of this peak predicted by the BTM occurs at a time instant of four pulse widths later than that of the two-temperature model. The phonon temperature predicted by the BTM is in good agreement with that of the Chen et al's [47] computation.

The BTM is applied to the problem of laser heating of Si film by varying different parameters and studying their impact on the thermal transport in nanometer size films. The categories considered for the parametric study are summarized in Table 5. It has been found that varying the film thickness of Si while keeping the laser fluence and pulse duration fixed does not have a significant effect on the peak carrier and phonon temperatures. Therefore, only two categories are considered. For each category several simulations are performed. In Category 1, the effect of laser pulse duration in the range of 0.05–10 ps is studied, keeping the thickness and the fluence fixed at 28 nm and 500 J/m², respectively. The Si film thickness of 28 nm is approximately ten times smaller than the phonon mean free path of 280 nm. In Category 2, the laser fluence is varied while maintaining the film thickness and pulse duration at 28 nm and 75 fs respectively. The pulse duration of 75 fs is smaller than the carrier-phonon collision time of 500 fs. The nanoscale film thickness, short pulse duration, and the relatively high fluence used in this study are chosen to create a strong non-equilibrium between the energy carriers.

4.2.3. Temporal characteristics of carrier-phonon non-equilibrium

Figure 10 shows the temporal evolution of carrier number density, carrier and phonon temperatures at the front surface of Si film for varying laser pulse duration, Category 1 of Table 5. For the all of cases considered in this study, it is found that the impact ionization term is negligible while the two-photon absorption term is significant only for values of laser fluence above 1000 J/m². From Figure 10 (a), it is observed that at very early times, the laser pulse is mainly supplying energy to the carriers, whereas it is not significantly increasing the number density of them. The number density of carriers exhibit a sharp increase at a time instant of four times the pulse duration. This figure shows that with increasing laser pulse duration, the peak value of carrier number density decreases. The rate of decrease of the carrier number density is the steepest for the largest pulse duration which can be attributed to the Auger recombination. With the increasing laser pulse duration, there is an increase in the carrier-carrier collisions resulting in the enhanced recombination of electron-hole pairs. From Figure 10 (b), it is observed that the carrier temperature starts to increase at a time instant of approximately twice the pulse duration, earlier than the increase in carrier number density. Due to the absorbed laser thermal energy, the carrier temperature increases rapidly to several thousands Kelvin as compared to the phonon temperature of few hundreds Kelvin. This is due to the heat capacity of carriers being several orders of magnitude smaller than the phonon heat capacity. For example, at room temperature the carrier heat capacity is approximately ten orders of magnitude smaller than the phonon heat capacity. During the initial time period extending to four times the pulse duration, the carriers are quite energetic. However, they do not transfer their energy to the phonons. Beyond this time, the carriers begin to transfer their energies to the phonons resulting in increase in the phonon temperatures. From Figure 10(b), it is depicted that the peak carrier temperature is the highest for the smallest pulse duration of 0.05 ps and decreases with increasing pulse duration. This is attributed to the strong non-equilibrium present for

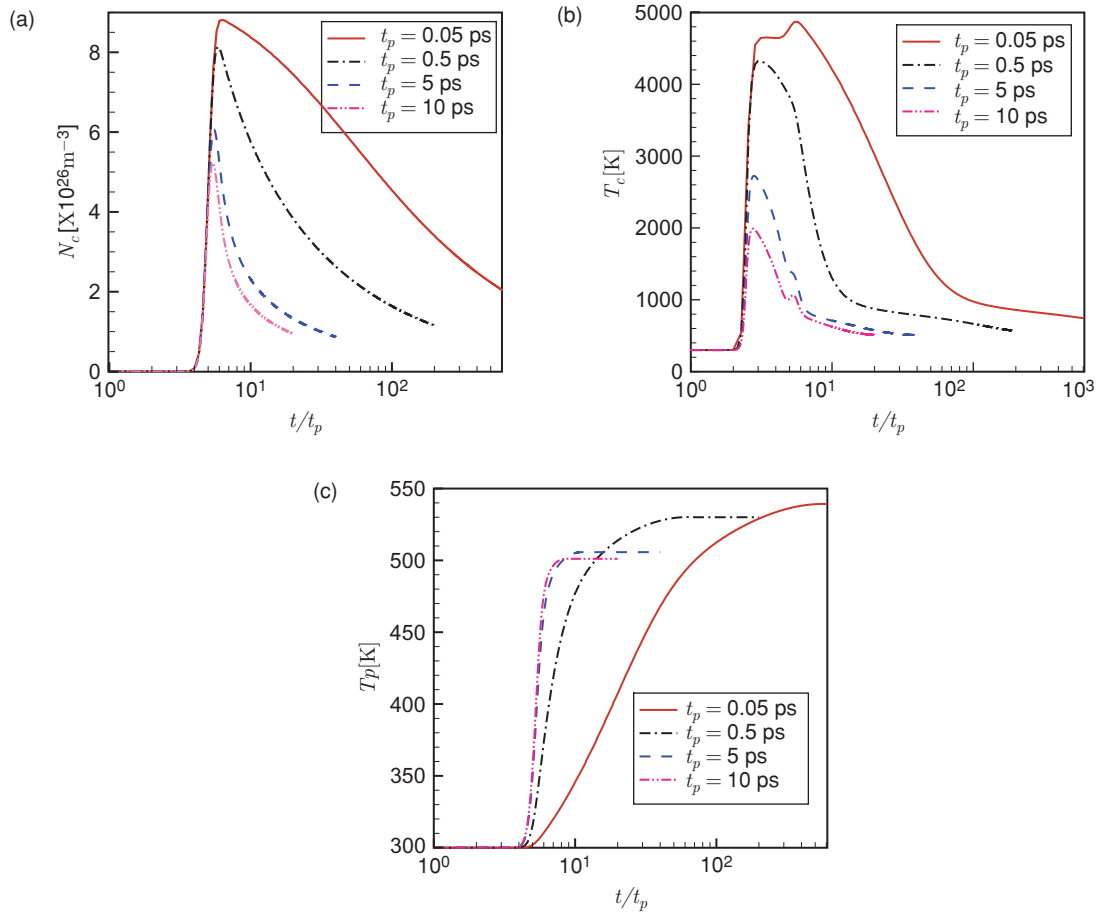


Figure 10. Temporal variation of (a) carrier number density (b) carrier temperature and (c) phonon temperature with pulse duration at the front surface for $L = 28$ nm and $\phi = 500$ J/m^2 .

small laser pulse duration cases. For the value of laser pulse duration of 0.05 ps, which is an order of magnitude smaller than the relaxation time of carriers, ballistic effects are dominant due to hyperbolic nature of carrier energy transport. For this case, the temporal evolution of T_c is qualitatively different from the other cases. For the pulse duration of 0.5 ps, only a single peak in carrier temperature is observed while a second peak due to Auger recombination appears for longer laser pulse durations as seen in Figure 10(b). The Auger recombination results in the transfer of bandgap energy into carrier energy leading to an increase in the carrier temperature which results in the second peak. In the BTM model, the carriers first transfer their energy to the optical phonons which then interact with acoustic phonons before reaching thermal equilibrium. From this figure, it is observed that the rate of increase in phonon temperature is the highest for the cases of larger pulse duration for which Auger effects are dominant. From Figure 10 (c), it is also observed that the peak phonon temperature decreases with increasing pulse duration.

Figure 11 shows the temporal evolution of carrier number density, carrier and phonon temperatures at the front surface of Si film for Category 2 of Table 5. From Figure 11 (a), it is observed that for fluences of 10 and 100 J/m^2 , the carrier number density increases and reaches constant values, since the Auger recombination is not dominant at small fluences. For higher laser fluences, the carrier number density increases rapidly and reaches a maximum after which it sharply decreases due to the

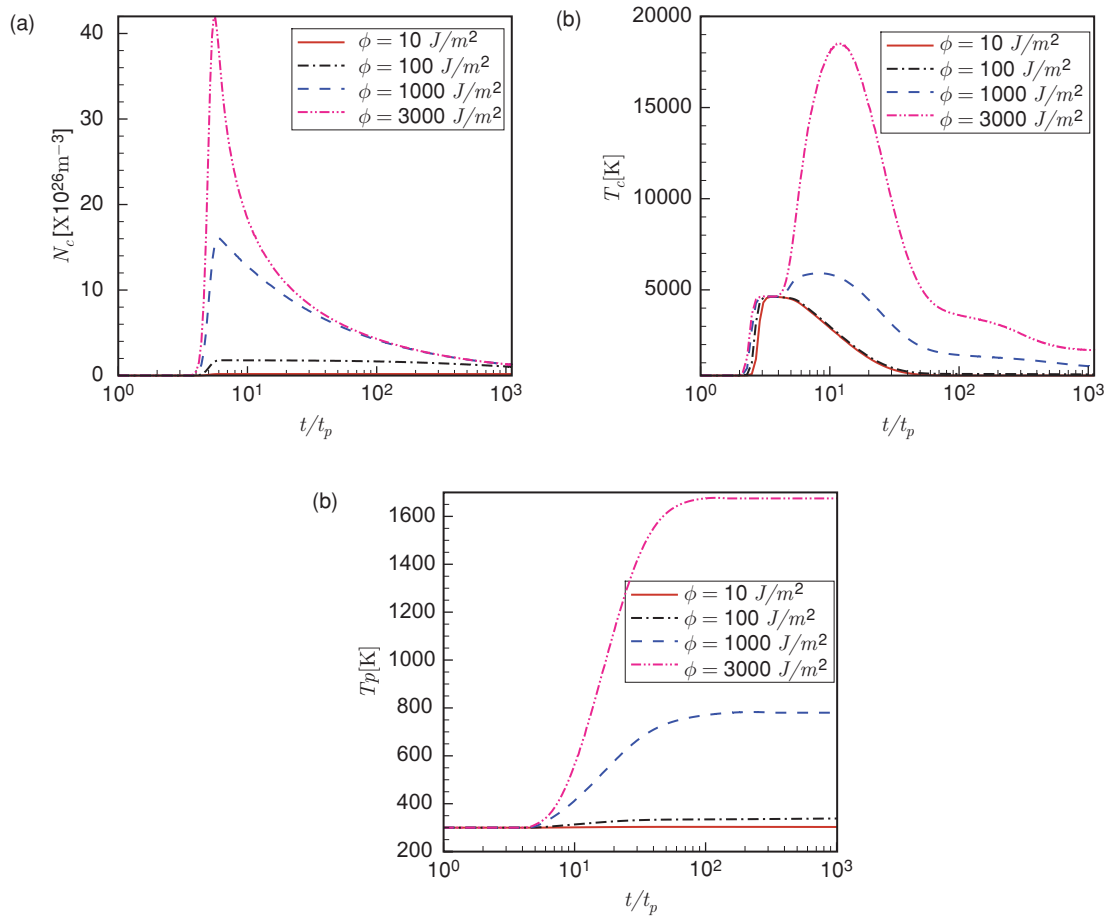


Figure 11. Temporal variation of (a) carrier number density (b) carrier temperature and (c) phonon temperature with laser fluence at the front surface for $L = 28$ nm and $t_p = 75$ fs.

Auger recombination which is proportional to the cubic power of carrier number density. Figure 11(b) shows the time evolution of carrier temperature for several values of laser fluences. The carrier temperature starts to increase ahead of the increase in the carrier number density. For fluences less than or equal to 100 J/m^2 , the carrier temperature decreases after reaching the peak. However, at higher fluences, due to the Auger recombination, a second peak higher than the first peak in carrier temperature is observed. The carrier energy is transferred to the phonons thus leading to an increase in the phonon temperature as seen in Figure 11(c). The carriers and phonons thermalize with each other and finally reach an equilibrium. From Figure 11 it is observed that the equilibrium temperature is a strong function of laser fluence, with the maximum value of equilibrium temperature observed for the largest fluence of 3000 J/m^2 . The equilibrium temperature for the case of largest laser fluence reaches values close to the melting temperature of 1680 K for Si while it is close to 300 K for the smallest fluence.

5. CONCLUSIONS

In this paper, energy transport in nanostructures has been studied using computational methods. The work is motivated by the ongoing technological revolution requiring device miniaturization and an accompanying understanding of the interesting phenomena that arise at these small length scales. The

ability to predict and manipulate thermal behavior at nanoscales will remain critical to further development in the areas of thermoelectrics and micro/nano electronics. The major conclusions of the numerical study are listed below:

5.1. Thermal transport in nanocomposites

The effective thermal conductivity of the nanocomposite is found to be dependent on the wire size, unlike for the bulk composite. The thermal conductivity decreases with decreasing wire size and for very small sizes or large atomic percentages, the wave effects have to be considered. The nanocomposite offers greater scalability than the superlattice due to phonon boundary scattering in multiple dimensions. Also, the nanocomposite is relatively more economical and suitable for thermoelectric applications that require tailored mechanical, electrical and thermal properties. It is found that for a fixed wire size, increasing the atomic percentage of the wire results in lower thermal conductivity of the nanocomposite. The thermal conductivity of $Bi_2Te_3-Sb_2Te_3$ nanocomposite for the wire size of 25 Å at 300 K is in the range of 0.034–0.74 depending on the interface specularity parameter and the atomic percentage. These factors combined with the prospect of enhancing the ZT make the $Bi_2Te_3-Sb_2Te_3$ nanocomposite a suitable alternative in efficient thermoelectric applications.

5.2. Carrier-phonon non-equilibrium in semiconductor films

In this study, the Boltzmann transport model (BTM) has been introduced to study the carrier-phonon non-equilibrium due to short pulsed laser interaction with thin Silicon films. The BTM results are compared with the previous computational results of two-temperature models. The BTM is then applied to perform a parametric study of the effect of the laser pulse duration and fluence on the non-equilibrium between the energy carriers for a fixed silicon film thickness of 28 nm. From the laser pulse duration study, it is observed that the maximum values of carrier number density, carrier temperature, and phonon temperature are the highest for the smallest pulse duration of 0.05 ps and decreases with increasing pulse duration. For longer laser pulse durations, a double peak due to Auger recombination is observed in the carrier temperature profile. The rate of increase in the phonon temperature is the highest for the cases with longer pulse duration where Auger effects are dominant. From the laser fluence study, it is observed that for fluences less than or equal to 100 J/m^2 , the carrier temperatures decrease continuously after attaining a peak. However, for higher fluences, due to the Auger recombination, a second peak higher than the first peak in carrier temperature is observed. The results of this study can help in addressing the non-equilibrium at the semiconductor-metal contacts of thermoelectric devices and in modeling ‘hot-spots’ in microelectronic devices.

6. SCOPE FOR FUTURE WORK

The area of modeling energy transport in nanostructures is still in its early stages. Future research in these fields may reveal more interesting phenomena and characteristics of these systems. Specific aspects of these future work areas are discussed below:

- 1) **Thermal transport in non uniform nanoparticle composites:** The present 3-D BTE simulations for modeling thermal transport in nanocomposites assume a uniform size and distribution of these nanoparticles in the host. The 3-D BTE solver can be extended to account for non uniform distribution of nanoparticles by introducing probability functions for describing the size and shape distributions of nanoparticles. This will account for the random distribution of nanoparticles that are used in actual thermoelectric/nano electronic applications.
- 2) **Full dispersion BTE simulation for nanocomposites:** The current simulations using Boltzmann transport equation for nanocomposites assume phonon gray medium approximation. More detailed simulations that can account for the complete dispersion relationships by considering the frequency or even wave vector dependent phonon propagation and phonon scattering can be introduced to determine the contribution of the different phonon modes to heat transfer.

- 3) **Electron-phonon non-equilibrium in nanocomposites:** Predicting the thermoelectric properties of nanocomposites has been a challenge since it involves solution of coupled BTEs describing both electron and phonon transport. The simulation schemes described in this paper can be extended for studying other transport properties, for example, the electrical conductivity and Seebeck coefficient in nanocomposites. This would help in designing efficient nanostructures for thermoelectric or nanoelectronic applications.
- 4) **Energy transport across nanostructure interfaces:** Understanding the fundamentals of energy transport across interfaces is the key to the breakthrough of developing novel materials for high efficiency energy conversion and thermal management. When the constituent materials across an interface are dissimilar, the energy carriers can be very different, and thus coupling among different energy carriers, for example electrons and phonons, can be very important. The simulation techniques developed for modeling electron-phonon non equilibrium in metals and semiconductors can be integrated to solve for electron-phonon non-equilibrium across interfaces of thermoelectric and microelectronic devices.

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