Thermal Transport in Nanostructures

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Transfer Report

September 15, 2005

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MC   Monte Carlo

BTE   Boltzmann Transport Equation

FET   Field Effect Transistor

HEMT   High Electron Mobility Transistor

HDE   Heat Diffusion Equation

AlGaAs Aluminium Gallium Arsenide

GaAs   Gallium Arsenide

InGaAs Indium Gallium Arsenide

GaN   Gallium Nitride

SiGe   Silicon-Germanium

SOI   Silicon-On-Insulator

IC   Integrated Circuits

C The specific heat

Abstract

The motivation behind the research on thermal transport in nanostructure is the continuous increase in the density of components of the integrated circuits leading to a detrimental effect on thermal management. As the number of components increase the heat dissipation becomes a major concern. The simple heat approximation of Fourier law is no longer valid at nanoscopic levels. Other laws such as the Boltzmann Transport Equation, Greens function and Drift diffusion have to be considered for the thermal analysis.

Thermal energy transport in nanostructures is based on the vibration of particles in the material; the particles oscillate in a harmonic way and they accept or lose only discrete amounts of energy. This energy is termed a phonon. Phonons like photons obey Bose-Einstein distribution of energy. Phonons can be treated as particles having a spherical shape and definite size to consider them for collisions in molecular dynamics simulations or in Monte Carlo simulation.

A literature review was made on phonons, their characteristics and on the papers based on the thermal transport in micro and nanostructures. The Monte Carlo method of simulation and molecular dynamics method of simulations were also studied. The C++ programming language was chosen to write the codes of the simulation as it is versatile and it has many standard libraries. Considerable time was spent on understanding the C++ codes. Before writing the codes for phonon simulation, an analogous system consisting of ideal gas was simulated using the molecular dynamics method to obtain a Maxwell-Boltzmann distribution.

Future work involves implementation of phonons in place of gas particles in the ideal gas simulation. This is then taken to the device level and implementing all the quantum effects. This report is divided into tree parts, literature review, ideal gas simulation and the future work.

Chapter 1

Introduction

The number of transistors in an integrated circuit has touched the one billion mark, and the rate of increase of these transistors is exponential with respect to time. This exponential increase in packing density creates tremendous increase in heat generation in the device. Dissipation of this heat has become a prime factor for the optimal performance of the semiconductor devices. A complete empirical exploration has not yet taken place in this area. Although there are advances in thermal metrology such as the 3ω method, time domain thermoreflectance, micro-fabricated test structures and the scanning thermal microscope [2], they do not suffice for the entire empirical exploration of thermal transport. There is an urgent requirement for supporting these experiments with the predictive device performance and reliable simulations. In order to obtain a reliable and a predictive simulation, a thorough understanding of physical principles of carrier transport at the nanolevel is essential.

Phonon transport is the main mechanism for heat transfer in semiconductor materials. The mean free path of a thermal phonon in silicon at room temperature is 300nm [3, 4] which is far greater than the channel length of modern day transistors. When the mean free path is comparable to the device scale, phonon travel is more ballistic, and bulk scattering is less frequent. If the mean free path is smaller than the device scale then the number of scattering events is high hence there will be thermal equilibrium [5]. As devices become smaller and smaller, the surface to volume ratio increases and boundary scattering begins to plays a larger

role in the thermal transport. In heterostructures interference reflection plays a critical role in determining the effective thermal conductance. When the device dimensions are comparable to phonon wavelengths, coherence effects come into picture [6]. These effects are not taken into account by the classical Fourier theory for heat conduction.

There are many laws which can account for many of these effects; Boltzmann transport equation (BTE), Greens function, drift diffusion equation, hydrodynamic energy transport equations,etc. There are some works on analytical solution of BTE of phonons using the Monte Carlo method of simulation[3, 7]. Molecular dynamics method of simulation has not been very popular because of its intense computational requirements. Only a few hundreds to thousands of particles can be considered for simulation with this method which is very few compared with the number of particles in a real system. The highest number of particles being used is one million at NASA Ames Research Centre by Leonardo Dagum to simulate hypersonic flow conditions [8]. With the availability of faster computers the number of particles in a real system can be matched with the number of particles in a simulation. It was useful to start with a simple system analogous to phonon transport for molecular dynamics method of simulation. An ideal gas system with elastic boundaries and neglecting multiple collisions was considered to obtain a Maxwell-Boltzmann distribution.

Chapter 2

Literature Review

2.1 Introduction

The understanding of many concepts of solid state physics is essential when dealing with the problems that arise in simulation of particles in nanostructures. A detailed literature review of the fundamentals of solid state physics are presented in this report. Fourier analysis, reciprocal lattice vectors, Brillouin zone, phonon definition, types of phonons, phonon heat capacity, density of states model, thermal resistivity of phonon gas and Umklapp processes are presented in detail. Fundamentals of the Monte Carlo method of simulation of phonons and electrons are reviewed, an introduction to molecular dynamics method of simulation is also presented in this chapter.

2.2   Lattice translation vectors

A crystal structure is a regular arrangement of particles in all directions. A lattice is a representation of the crystal structure but with out the actual particles, in other words a periodic array of points. The lattice is defined by three translation vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ such that the atomic arrangement looks the same in every respect when viewed from the point $\mathbf{r}$ as when viewed from the point

$$r' = r + u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3 \qquad (2.1)$$

where u_1, u_2, u_3 are arbitrary integers.

There are many operations carried out on the lattice, including translation operation, point operation (rotation and reflection) and the combination of both translation and point operations. A lattice translation operation is defined as the displacement of a crystal by a crystal translation vector.

$$T = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3 \qquad (2.2)$$

Any two lattice points are connected by this form of vector.

2.3   Types of Lattices

There are 14 different lattice types from the seven basic types: triclinic, monoclinic, orthorhombic, tetragonal, cubic, trigonal and hexagonal. There are three different lattices in the cubic lattice: simple cubic (SC), body centered lattice (BCC) and face centered cubic lattice (FCC). There is a special kind of cubic lattice crystal structure known as the diamond structure. It has tetrahedral bonding characteristics; each atom has 4 nearest neighbors and 12 next neighbours. Carbon, silicon, germanium and tin all exhibit this kind of crystal lattice structure. The figure

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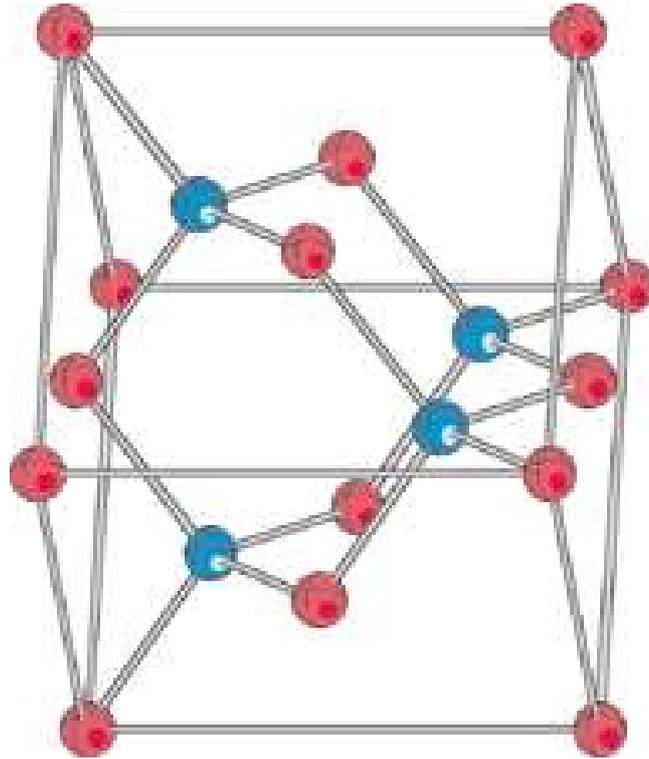
Figure 2.1: Diamond Crystal structure

2.2 is a diamond crystal structure of silicon. The table 2.1 lists all the lattice types [1, 9, 10].

2.4 Fourier Analysis

Fourier analysis is an important tool when dealing with electron density. Electron density is a periodic function of $\mathbf{r}$ with the periods a_1, a_2, a_3.

n($\mathbf{r}$+$\mathbf{T}$)=n($\mathbf{r}$).

The function $n(x)$ with period a in the x direction may be expanded in a Fourier series of sines and cosines as follows:

$$n(x) = n_0 + \sum_{p>0}[C_p cos(2\pi px/a) + S_p sin(2\pi px/a)] \tag{2.3}$$

Table 2.1: Different lattice types.

System	Number of Lattice	axes and angles restriction
triclinic	1	$a_1 \neq a_2 \neq a_3, \alpha \neq \beta \neq \gamma$
monoclinic	2	$a_1 \neq a_2 \neq a_3, \alpha = \gamma = 90 \neq \beta$
orthorhombic	4	$a_1 \neq a_2 \neq a_3, \alpha = \beta = \gamma = 90$
tetragonal	2	$a_1 = a_2 \neq a_3, \alpha = \beta = \gamma = 90$
simple cubic	3	$a_1 = a_2 = a_3, \alpha = \beta = \gamma = 90$
trigonal	1	$a_1 = a_2 = a_3, \alpha = \beta = \gamma \textlangle 120, \neq 90$
hexagonal	1	$a_1 = a_2 \neq a_3, \alpha = \beta = 90 \ \gamma = 120$

where p is a positive integer and Cp and Sp are constants called the Fourier coefficients of expansion. The factor $2\pi/a$ ensures that $n(x)$ has a period a. It can be written as follows in compact form.

$$n(x) = \sum_{p} n_p exp(i2\pi px/a) \tag{2.4}$$

The Fourier analysis of a periodic function $n(\mathbf{r})$ in three dimensions can be written as

$$n(\mathbf{r}) = \sum_{G} n_G exp(i\mathbf{G}.\mathbf{r}) \tag{2.5}$$

2.5   Reciprocal Lattice Vectors

Every crystal structure has two lattices associated with it; the crystal lattice and the reciprocal lattice. The diffraction pattern of the crystal lattice is the map of the reciprocal crystal lattice. The two lattices are related by the following expressions in equation.

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 . \mathbf{a}_2 \times \mathbf{a}_3}; \tag{2.6}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 . \mathbf{a}_2 \times \mathbf{a}_3}; \tag{2.7}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 . \mathbf{a}_2 \times \mathbf{a}_3} \tag{2.8}$$

where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are primitive vectors of the crystal lattice and $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the primitive vectors of the reciprocal lattice

A reciprocal lattice is mapped by the following equation

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 \tag{2.9}$$

where v_1, v_2, v_3 are integers. A vector of this type is a reciprocal vector.

2.6   Brillouin Zones

When a number of vectors are drawn from any point to the various lattices and perpendicular bisectors are drawn for those vectors, the smallest enclosed area is the Wigner-Seitz primitive cell. It is also called as first Brillouin Zone when the construction is made in the reciprocal lattice. The figure 2.2 shows the first Brillouin Zone [1]
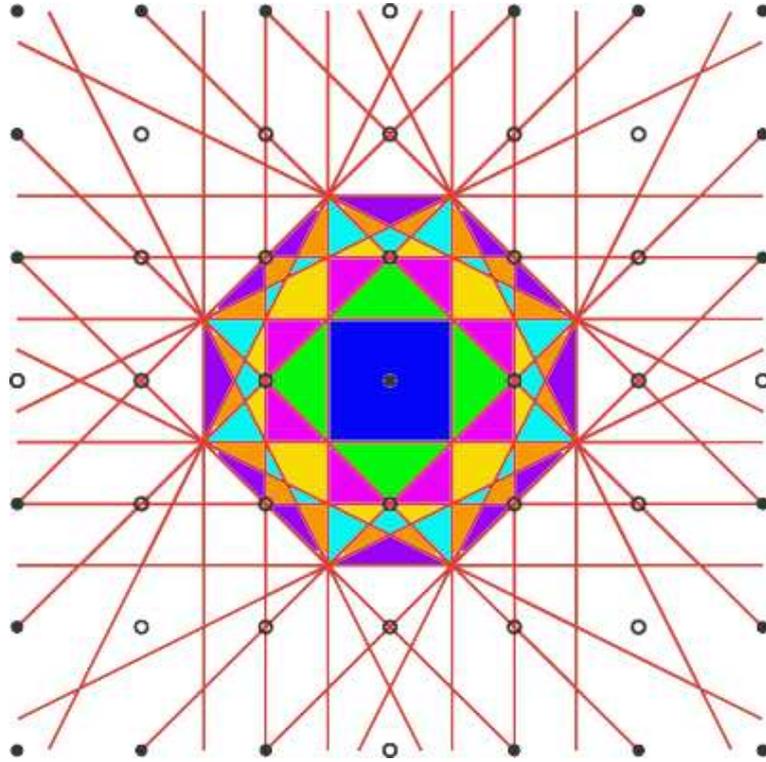
Figure 2.2: Brillouin Zone

The plot of the ω and the wave vector **K** shows the first Brillouin zone graphically[1]. **K** will have a range of $\frac{-\pi}{a}$ to $\frac{\pi}{a}$. Values of **K** outside the first Brillouin zone reproduce the lattice motions described by the values within the $\frac{-\pi}{a}$ to $\frac{\pi}{a}$ limits. This means we can treat the **K** values outside these limits by subtracting the integer multiples of $\frac{2\pi}{a}$ that will give wave vectors inside these limits.

The shortest wavelength a phonon can have is $2a$. The phonon energy is directly proportional to the frequency of oscillation. The phonon energy is governed by Bose-Einstein statistics which means that the energy of a particular mode of oscillation is *nhv* where *h* is Planck's constant, *v*

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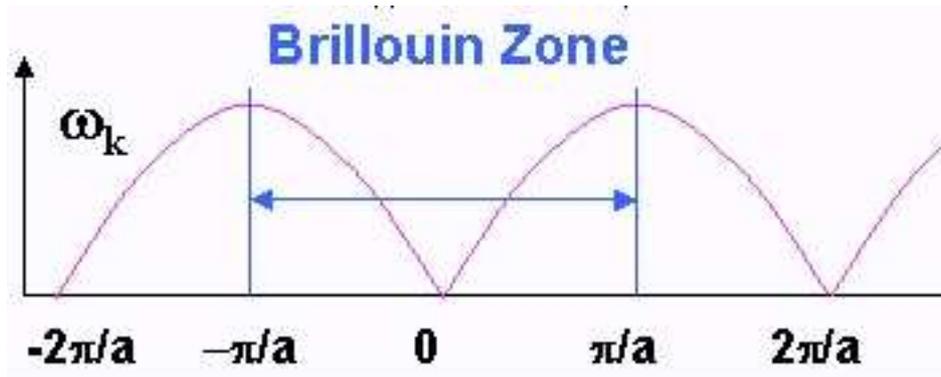
Figure 2.3: Graphical representation of Brillouin Zone

is the frequency and *n* is an integer whose value at temperature T is given by

$$n = (\exp^{\frac{h\nu}{kT}} - 1)^{-1} \qquad (2.10)$$

The Brillouin zones for different lattice structures will be different. The Brillouin zone for a simple cubic lattice structure is as shown below in figure 2.4 [1].
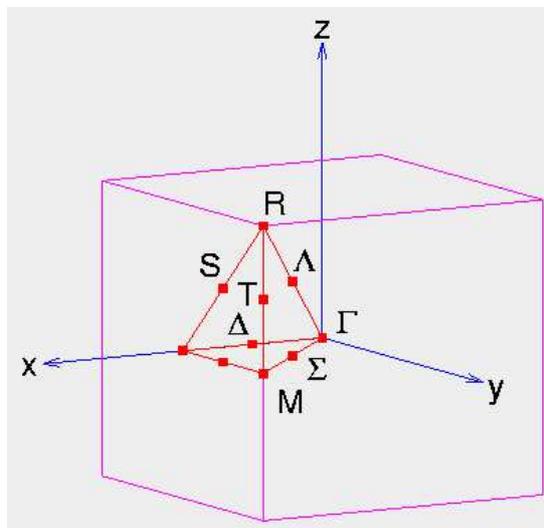
Figure 2.4: The Brillouin zone for simple cubic lattice structure

The Brillouin zone for a body centered lattice structure is as shown in figure 2.5 [1]
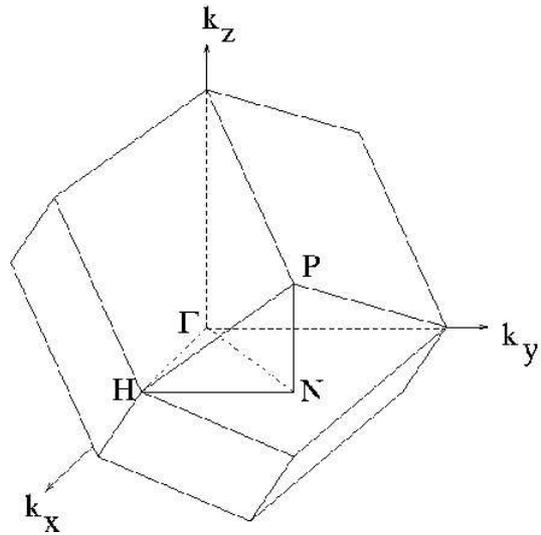
Figure 2.5: The Brillouin zone for a Body Centred Cubic lattice structure

The Brillouin zone for a face centered lattice structure is as shown in the figure 2.6 [1]
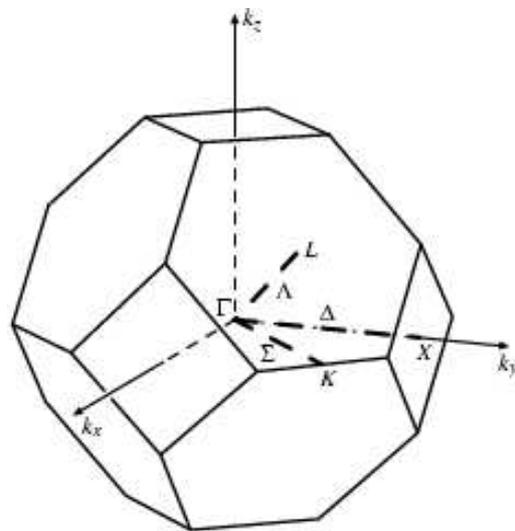
Figure 2.6: The Brillouin zone for a Face Centered Cubic lattice structure

2.7   Types of Phonons

Phonons can be classified in two ways, one based on the direction of the vibration with respect to the crystal lattice and the other is based on the frequency and the wavelength. The type of phonons classified on the basis of direction of oscillation are longitudinal and transverse phonons. The longitudinal phonons oscillate in the direction of propagation and the transverse phonons oscillate in the direction perpendicular to the direction of propagation. The types of phonons classified based on the frequency and the wavelength are acoustic and optical phonons. The acoustic phonons are those whose frequencies become small at the longer wavelengths and which travel at the velocity of sound in the lattice. Optical phonons have a minimum frequency even at very long wavelengths and they occur only in crystals which have more than one atom per unit cell.

The figure 2.7 and 2.8 shows the acoustic and optical phonons in monatomic and diatomic crystals respectively.
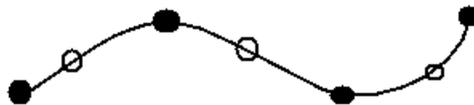
Figure 2.7: Acoustic Phonon [1]
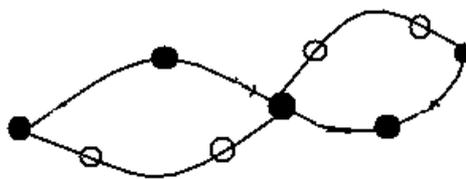
Figure 2.8: Optical Phonon[1]

The dispersion curves for all types of phonons is shown in the figure 2.9 [1].
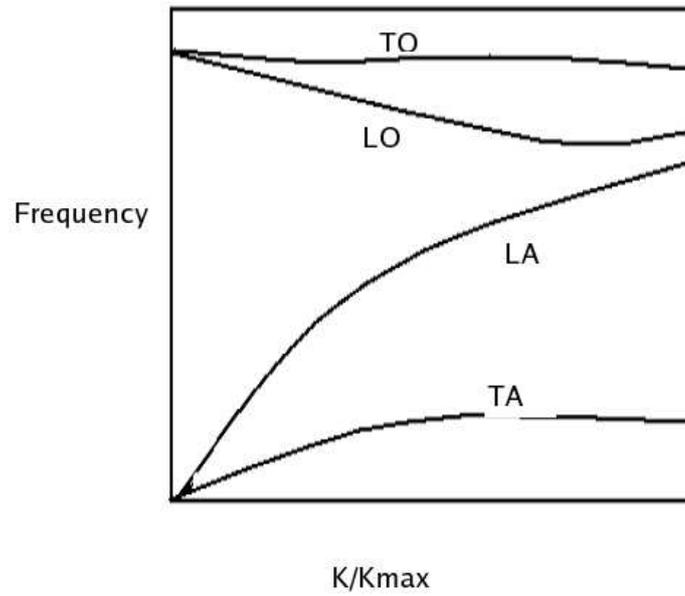
Figure 2.9: Dispersion relation for all types of phonons

2.8   Dispersion Curve

The dispersion relation between the frequency of the phonon ω and the wave vector K is given by

$$\omega_k = \sqrt{2\omega^2(1 - \cos(ka))} \tag{2.11}$$

The speed of the phonon is the speed of the sound in the crystal and is equal to the slope of the curve in the above graph. At the low values of k the dispersion relation is almost linear and speed of the sound is ωa which is almost independent of the phonon frequency.
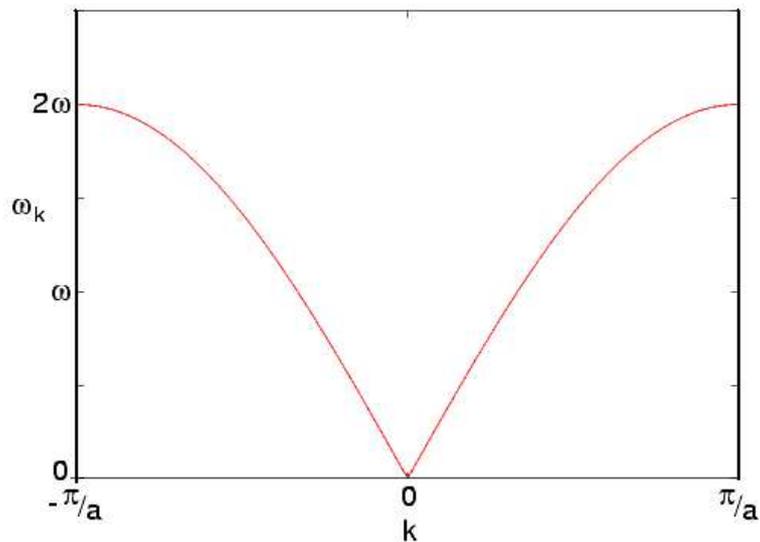
Figure 2.10: The Phonon dispersion relation[1]

2.9   Phonon Momentum

A phonon does not actually have a momentum but it interacts with the other particles like protons, electrons, etc as if it has a momentum equal to $\hbar K$ called the crystal momentum. Phonons do not have a momentum because their coordinates involve relative coordinates; the term exp($iNKa$) in equation 2.13 becomes 1 when s is run over N atoms. Hence they do not carry linear momentum. The phonon dispersion relation is mainly determined by the inelastic scattering of neutrons with the emission or absorption of a phonon.

$$\rho = M(d/dt)\Sigma u_s \tag{2.12}$$

$$\rho = M(d/dt)\sum_s exp(isKa)u_s = M(du/dt)[1 - exp(iNKa)]/[1 - exp(iKa)] \tag{2.13}$$

2.10 Phonon Heat Capacity

Heat capacity at constant volume is more fundamental than heat capacity at constant pressure and is widely used. Heat capacity at constant volume is defined by $C_v = (dU/dT)_v$ where U is the energy and T is the temperature. The contribution of phonons to the heat capacity of the crystal is called lattice heat capacity which is denoted by C_{lat}. The total vibrational energy of a phonon at a temperature t in a crystal may be written as the sum of energies over all the phonon modes[5].

$$EV = \sum_k \sum_p U_{K,p} = \sum_k \sum_p \left(\langle n \rangle + \frac{1}{2}\right)\hbar\omega \tag{2.14}$$

where $\langle n \rangle$ is the thermal equilibrium occupancy of phonons of wave vector K and polarisation p. The form of $\langle n \rangle$ is given by the Planck distribution function.

$$\langle n \rangle = \frac{1}{exp\left[\frac{\hbar\omega}{k_B T}\right] - 1} \tag{2.15}$$

2.11 Thermal Conductivity

The thermal conductivity coefficient K of a solid is defined by:

$$j_U = -KdT/dx \tag{2.16}$$

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where j_U is the flux of thermal energy, or the energy transmitted across unit area per unit time [1].

The thermal conductivity in any material is a random process; heat does not just enter at one end and exit at the other end of a material without suffering any collisions rather it diffuses in the material suffering constant collisions, hence thermal conductivity depends on the temperature gradient not just temperature difference. The expression for the thermal conductivity K is given by

$$K = \frac{1}{3}Cvl \tag{2.17}$$

where C is the heat capacity per unit volume, v is the average particle velocity, and l is the mean free path of a particle between collisions.

2.12 Thermal Resistivity

The phonon mean free path is determined predominatly by two factors; geometrical scattering and scattering by other phonons. There would be no mechanism for collisions between the phonons if the attraction force between the atoms were purely harmonic. The mean free path would only depend on collisions of phonons with the boundary and with lattice imperfections. An anharmonic lattice interaction provides a coupling between different phonons which limit the value of the mean free path. At high temperatures the number of exited phonons is proportional the temperature T. The collision frequency of a given phonon should be proportional to the number of phonons with which it can collide. Hence the mean free path l is inversely proportional to the temperature T.

2.13   Umklapp Processes

The important three phonon processes that cause thermal resistivity are of the form given in 2.18

$$\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3 + \mathbf{G} \qquad (2.18)$$

where $\mathbf{G}$ is a reciprocal lattice vector.

There can be examples of wave interaction processes in the crystals for which the total wave vector change need not be zero, but may be a reciprocal lattice vector. The meaningful phonon K always lie in the first Brillouin zone, so any longer K produced in a collision must be brought back into the first Brillouin zone by addition of a reciprocal lattice vector G. A collision of two phonons with the negative wave vectors K can be an Umklapp process create a phonon with the positive wave vector K. This process is also called a U process.
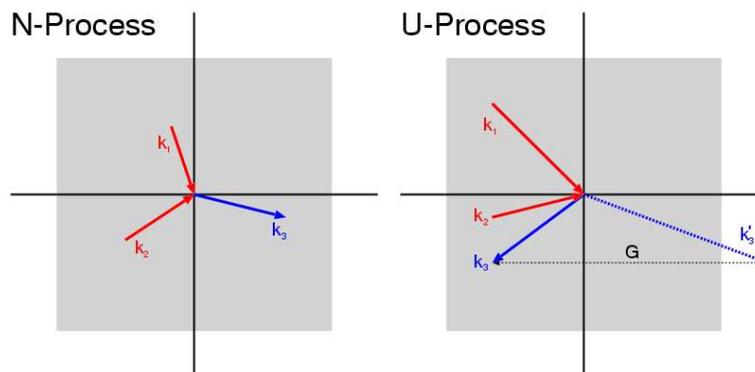

Figure 2.11: Normal $\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3$ and Umklapp $\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3 + \mathbf{G}$ phonon collision processes in a 2-dimensional square lattice

2.14   Fundamentals of Monte Carlo simulation

The Monte Carlo (MC) method is the branch of experimental mathematics that uses random numbers. MC calculations can be considered as simulation experiments. The simulation results have to be interpret in physical terms for better understanding of the problem. Its application is in wide range of fields from casinos to simulation of phonon transport in nanostructures[7]. The application of MC can be divided into two major groups; direct simulation of statistical problems and simulation of a deterministic problem with a statistical interpretation which mainly involves solution of a well defined mathematical equation describing a particular problem. The majority of real cases are a mixture of both the kind of applications. The application of MC simulation to the transport equations is a good example. Transport problems are basically statistical in nature but they are also described by mathematical equation to some extent of accuracy. The application of MC technique to high field transport in semiconductors was first introduced in a semiconductor conference in 1966 by Kurosawa [11, 12]. Since then the MC technique became popular in the field of transport theories in semiconductor devices.

2.14.1   Random Number Generation

Random number generation is an important part of the MC technique. The most popular and simplest method of generating a random number with uniform distribution is to use a recursive formula.

$$x_i = a x_{(i-1)} + c \quad (\text{modulo} \quad m) \tag{2.19}$$

All integers between 0 and $m-1$, used as $r = x/m$

In the above equation the next number makes use of the previous one to generate a random number. The sequence has to start with a freely chosen number x_0 known as seed. The numbers generated by equation 2.19 are not truly random in actual sense as in a sequence of random numbers it should not be possible to predict the next number, but it is possible in the equation 2.19.

The other method of random number generation is by transformation of the distribution generated from the recursion formula 2.19. Let $f(t)$ be a single-valued function of the variable t defined for $t_s < t < t_f - f(t)$ [13] should have the properties that

$$f(t_1) < f(t_2) \quad \text{for } t_1 < t_2 \tag{2.20}$$

and

$$\int_{t_s}^{t_f} f(t)dt = 1 \tag{2.21}$$

condition 2.20 says that $f(t)$ is a monotonously growing function of the independent variable t and condition 2.21 says that the function can be normalised.

If r_i is a flat random number of uniform distribution then r' is a number of stochastic density.

2.14.2   Simulation Procedure

In most of the Monte Carlo simulations, first the geometry of the system is defined considering the boundary contacts, air-boundary interface, etc. then the initial conditions such as position, velocity, potential, field etc are assigned. Position and velocities are randomly assigned using certain distribution. The time cycle is defined which is used for updating the velocity, position and other properties after each cycle. Free flight, acceleration (not for phonons), displacement is calculated before every scattering event. The scattering mechanism is determined depending on the probability rate of each type of scattering process. In some models the electron-electron scattering is considered independently similar to self scattering mechanism[14]. Now all the properties of the system i.e. velocity, position, potential, field etc are calculated using appropriate laws.

The Monte Carlo method of simulation is a well established technique and it is not computationally very intense, hence this technique is quite popular in device simulations.

2.15   Molecular Dynamics Method

Molecular dynamics is the study of motion of molecules (particles) to gain a deeper understanding of many chemical reactions, fluid flow, phase transition and other physical phenomenon such as heat transfer, droplet formation,etc. Much of the molecular dynamics method uses simple Newtonian mechanics. Scientific visualisation is important for understanding the results of a molecular dynamics method. The history of position and velocity of millions of particles have to be calculated and they need to be updated after every time step. The computations are quite simple but are many in number. To achieve greater accuracy the time steps needs to be quite small. The amount of computation at each step can be quite extensive. Thus it consumes large amount of machine cycles.

There are mainly three different models of molecular dynamics: Hooke's Law model, Lennard-Jones model and hard sphere model[8, 15]. In Hooke's model the force acts as if the particles were connected to their neighbours by a spring. The Lennard-Jones model takes into account the large repulsive force at very short interparticle distances, attractive forces at larger distances and extremely weak attractive forces at very large distances. And in the hard sphere model, the particles are treated similar to billiard balls- they bounce off each other when they are a certain distance apart, otherwise they do not interact. Solving the equations of motion for a hard sphere model requires solving simple geometric problems. It is very simple in one and two dimensions, but a three dimensional approach requires the knowledge of vector analysis. With Hooke's model and Lennard-Jones model we must solve a system of differential equations using Euler's and Verlet's method.

There are some basic assumptions in the molecular dynamics method, they are:-

a) each particle is treated as a point mass;

b) simple force rules describe the interactions between atoms ie the total force acting on a particle due to the other particles is the sum of the forces between pairs of particles;

$$f_i = \sum_{j=1, j\neq i}^{n} f_{i,j} \qquad (2.22)$$

c) Newton's equations are integrated to advance the atomic positions and velocities;

d) thermodynamic statistics are extracted from the atoms.

The hard sphere molecular dynamics method is preferred over the other two models because, it is easy to implement all types of phonon scattering mechanism using this molecular dynamics method. The hard sphere molecular dynamics method is explained in detail.

The hard sphere method assumes the constituent particle as a spheres traveling at a constant speed and in straight line before the collision. Determining the sequence of the collision is computationally intense. If the particles collide head on and if we consider them only in one dimension then, conservation of momentum equation 2.23 and conservation of energy equation 2.24can solve for the resulting new position and velocity[16].

$$m_1\mathbf{u}_{1old} + m_2\mathbf{u}_{2old} = m_1\mathbf{u}_{1new} + m_2\mathbf{u}_{2new} \qquad (2.23)$$

$$m_1\mathbf{u}_{1old}^2 + m_2\mathbf{u}_{2old}^2 = m_1\mathbf{u}_{1new}^2 + m_2\mathbf{u}_{2new}^2 \qquad (2.24)$$

In three dimensions the particles need not collide head on, it can be oblique as illustrated in the figure 2.12. In an oblique collision, the interaction between the particles is along the line drawn between the centres of the particles at the instant of the collision. There is no force exerted on the particles in the plane tangent to the particles at impact. Only a component of the velocity is exchanged along the line joining the centres of the two particles. This is illustrated in the figure 2.13.

The main step in updating the velocities is determining which particle is going to collide next. The test to determine if two particles collide is divided into two steps; one to test if the particles are approaching each other and the second is to test if the particles which are approaching each
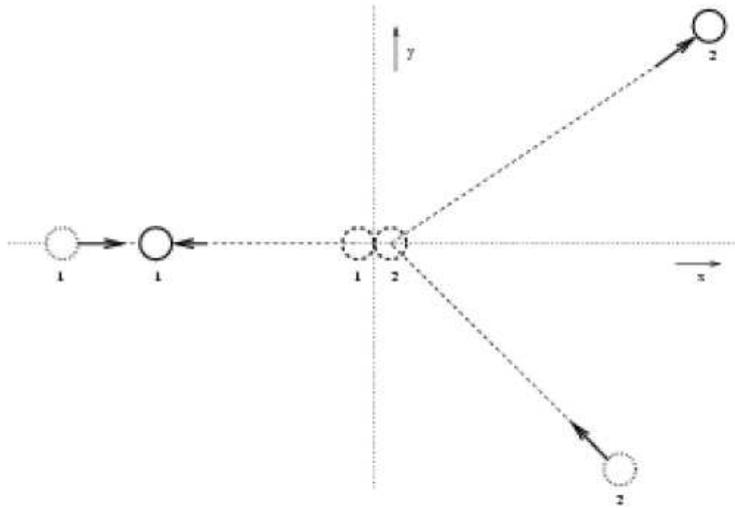
Figure 2.12: Oblique collision

other will come closest to the collision distance. The particles approach each other if the dot product of the relative velocity and relative position of two particles is less than zero shown in equation 2.27. The relative positions and relative velocities can be calculated and represented in 2.25 and 2.26 respectively.

$$\mathbf{u}_{i,j} = \mathbf{u}_1 - \mathbf{u}_2 \qquad (2.25)$$

$$\mathbf{r}_{i,j} = \mathbf{r}_1 - \mathbf{r}_2 \qquad (2.26)$$

$$\mathbf{r}_{i,j} \cdot \mathbf{v}_{i,j} < 0 \qquad (2.27)$$

The other step to determine if two particles collide or not is by the condition 2.28

$$\|\mathbf{b}_{i,j}\| = \sigma; \qquad (2.28)$$

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Figure 2.13: Velocity exchange between two particles in three dimensions

where

$$\|\mathbf{b}_{i,j}\|^2 = \|\mathbf{r}_{i,j}\|^2 - \left(\frac{\mathbf{r}_{i,j}\cdot\mathbf{v}_{i,j}}{\mathbf{v}_{i,j}}\right)^2 \tag{2.29}$$
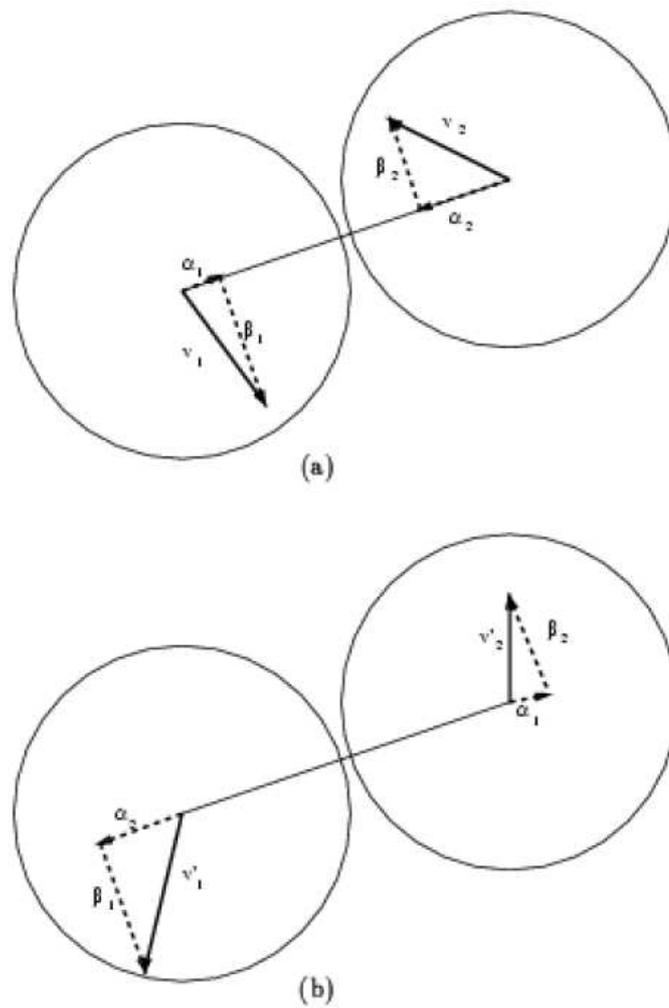
With some simple geometrical consideration from the figure 2.30, the time of collision [17]can be calculated by the equation 2.14
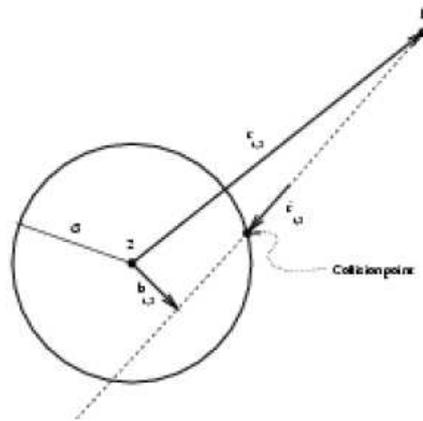
Figure 2.14: Time of collision is the time taken by particle 1 to reach the collision point

$$t_{ij} = -\frac{1}{\|\mathbf{v}_{ij}\|}\left(\frac{\mathbf{r}_{ij}\cdot\mathbf{v}_{ij}}{\|\mathbf{v}_{ij}\|} + (D^2 - \|\mathbf{b}_{ij}\|^2)^{1/2}\right) \tag{2.30}$$

The equation2.30 can be understood by observing the second term $\left(\frac{\mathbf{r}_{ij}\cdot\mathbf{v}_{ij}}{\|v_{ij}\|} + (D^2 - \|b_{ij}\|^2)^{1/2}\right)$ as the distance traversed in the direction of $\mathbf{v}_{i,j}$ before the collision.

The change in velocity is calculated after the collision. There is no change in velocity in the plane tangent to the spheres at the collision point; the velocity changes only in the direction of the line between the centres of the particle as illustrated in figure 2.15.

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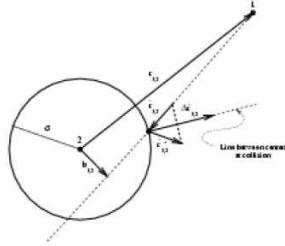
Figure 2.15: Change in velocity is only in the direction of line between the centre of the particles

Thus change in velocity is given by the equation 2.31.

$$\Delta\mathbf{v}_i = -\Delta\mathbf{v}_j = \frac{(\mathbf{r}_{ij}.\mathbf{v}_{ij})\mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|^2} \tag{2.31}$$

The resultant velocity of both the particles is given by equations 2.32 and 2.33

$$\mathbf{v}_i = \mathbf{v}_i + \Delta\mathbf{v}_i \tag{2.32}$$

$$\mathbf{v}_j = \mathbf{v}_j - \Delta\mathbf{v}_j \tag{2.33}$$

Chapter 3

Ideal Gas Simulation

3.1 Introduction

Ideal gas system is the simplest system to consider for simulation using molecular dynamics as there are well established laws for the velocity distribution, energy distribution, boundary conditions, etc. There are some basic assumptions when an ideal gas system is considered [18]. They are:

a) the gas molecules have no volume.

b) there are no forces between the gas molecules.

c) no energy is lost in collision of molecules; the impacts are completely elastic.

d) the temperature of a gas is the average kinetic energy of all of the molecules.

e) the interaction is only between a pair of particles(there are no multiple collision)

f) the boundaries of the system are elastic(the particle leaving the system through one wall enters through the other wall with the same velocity).

The ideal gas is governed by an equation known as ideal gas equation 3.1.

$$PV = nRT \tag{3.1}$$

where P is pressure, V is volume of the gas, n is number of moles, R is the gas constant, T is the temperature

The average kinetic energy of the ideal gas is given by the equation 3.2

$$KE_{avg} = \frac{3}{2}kT \tag{3.2}$$

where k is the Boltzmann constant and T is the temperature.

The root mean square velocity of the molecules is given by 3.3

$$v_{rms} = \sqrt{\frac{3RT}{M}} \tag{3.3}$$

where M is the molar mass.

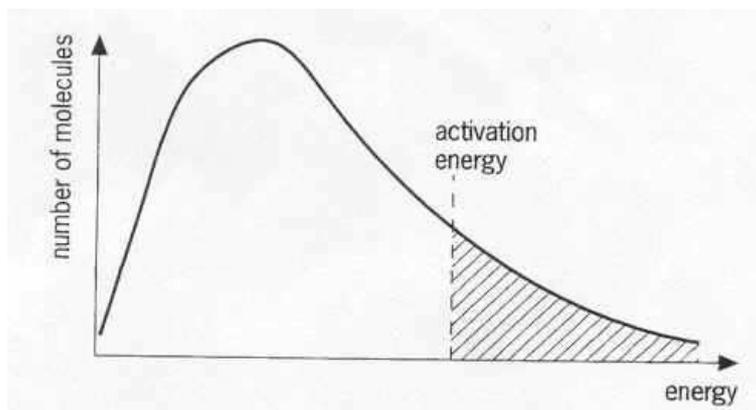The Maxwell-Boltzmann energy distribution is shown in the figure 3.1

Figure 3.1: Maxwell-Boltzmann energy distribution

3.2   Method Applied

A system consisting of 1000 identical particles in a 3 dimensional volume V is considered. The interactions between the spheres is hard core interaction: u(r)=0 for $r > \sigma$ and u(r)=∞ for $r < \sigma$. Where r is the separation of the centers of a pair of particles and σ is the collision diameter. The volume V is a box with the penetrable wall and particles are constrained in such a way that their number in the box remains constant. The particles which leave the wall through one end are placed in the box with unchanged speed but with having opposite direction. The position of the particle is changed based which boundary it has crossed. For the right and the upper boundaries the particles position is changed according to equations 3.4 and 3.5, and for the left and the lower boundary the particle's position is changed according to the equation 3.6 and 3.7. This is illustrated in the figure 3.2. For all the particles positions and velocities are randomized first using the random number generator. The positions and velocities of all the particles relative to other particles are calculated using the equations 2.25 and 2.26. This means each particle will have N(N-1)/2 relative velocities and N(N-1)/2 relative positions.

The particles are approaching each other if the dot product of the relative velocity and relative positions of the particles is less than zero, otherwise the particles are moving away from each other. The particles will collide each other if the equation 2.28 is satisfied, otherwise the collision time is treated as ∞. For the particles colliding each other, collision time called t_{ij} is calculated which is equal to the time required to reach the separation of D; D being the diameter of the particles.

$$P(x, y, z) = 2P(boundary - right - coordinates) \quad - \quad P(x, y, z) \tag{3.4}$$

$$P(x, y, z) = 2P(boundary - top - coordinates) \quad - \quad P(x, y, z) \tag{3.5}$$

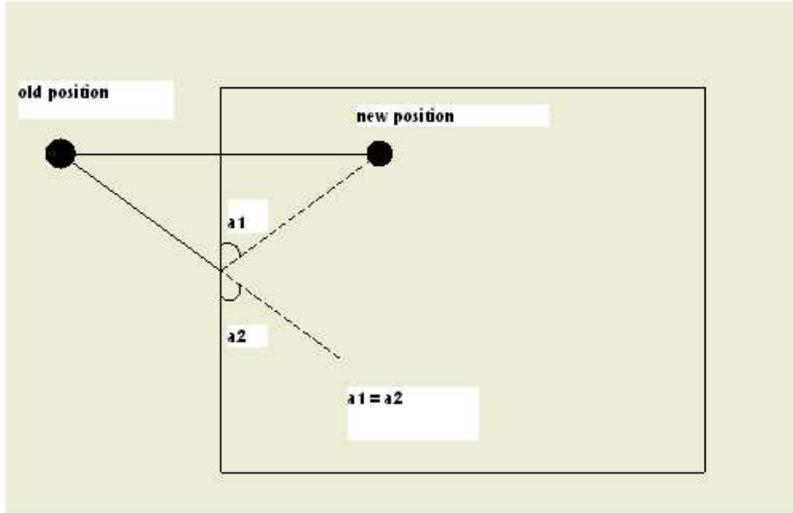$$P(x, y, z) = 2P(boundary - left - coordinates) \quad + \quad P(x, y, z) \tag{3.6}$$

Figure 3.2: Elastic boundary illustration

$$P(x, y, z) = 2P(boundary - bottom - coordinates) \quad + \quad P(x, y, z) \tag{3.7}$$

The collision time of all the colliding particles is put in a list and sorted in an ascending order. The first element of the collision-time list or the lowest collision time, corresponds to the particles which will collide first. Once these particles collide their new velocities are calculated using the equations 2.32, 2.33. The new positions of all the particles are calculated using the equations 3.8. The lowest collision time is subtracted with all the members of the collision-time list. Now the collided particles are again checked with all other particles for collision. If their collision time with any other particle is less than the highest collision time in the list then it is added to collision-time list. After every collision velocity, positions are updated. This process is repeated till the equilibrium is attained. The energy of all the particles is calculate using the formula 3.9. A graph of energy is plotted against the number of particles. This graph is then compared with the Maxwell-Boltzmann equation. The mass of the particle can be calculated using the equation 3.10. For simplicity the gas considered for the simulation is hydrogen. The mass of one atom of hydrogen is 1.66×10^{-24} kg.

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$$\mathbf{P}_{new} = \mathbf{P} + \mathbf{v}_{new}(t_{collision}) \tag{3.8}$$

$$E = \frac{m\|\mathbf{v}\|^2}{2} \tag{3.9}$$

$$m_{hydrogenparticle} = \frac{atomic\,mass\,unit_{hydrogen}}{Avogadro\,Number} \tag{3.10}$$

3.3   Results

The simulations were run with varying particle numbers, initial velocity of the particle and the size of the block. Since the energy of each particle is too small to represent in the graph, the x-axis is scaled down to the value of the mass of a hydrogen atom(1.66×10^{-24}). Figure 3.3 shows the simulation of 800 particles run for 100 iterations.
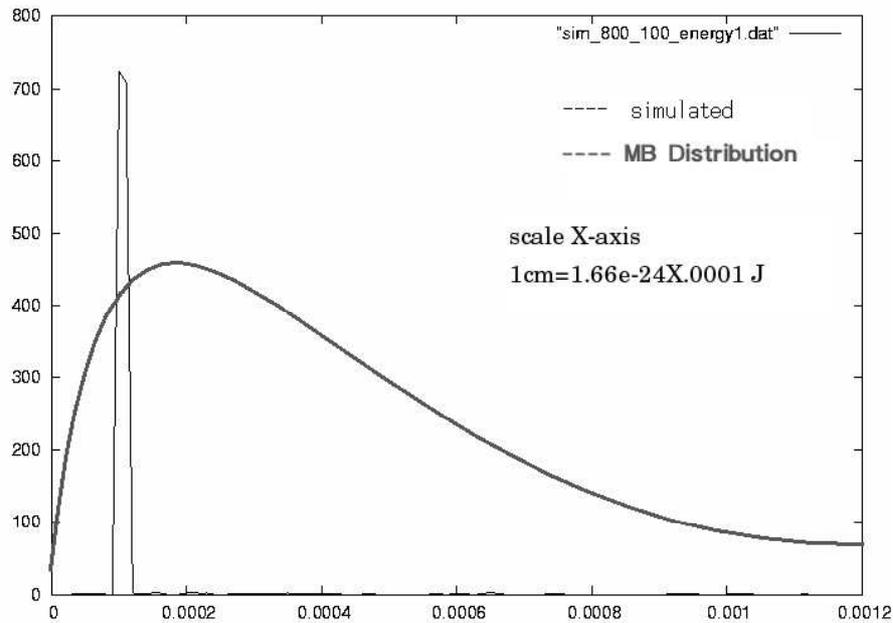

Figure 3.3: simulation of 800 particles over 100 iterations

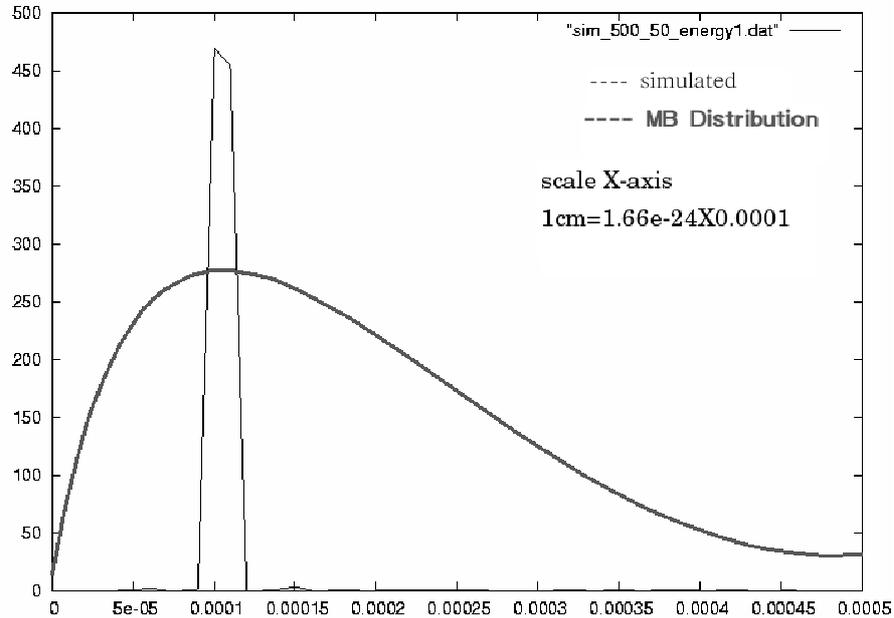Figure 3.4 shows the simulation of 500 particles run for 50 iterations

Figure 3.4: simulation of 500 particles over 50 iterations

3.4 Conclusion

The molecular dynamics method of simulation was applied to an ideal gas to check if the algorithm works. The algorithm was not just devised to simulate ideal gas, it considered three dimensions and it considered that the entire system is divided into periodic blocks, and the particles leaving one block enters the adjoining block thus maintaining the same number of particle when any block is considered. All these consideration are very useful when the algorithm will be applied to phonon simulation. The graph of energy distribution against number of particles did not exactly match the Maxwell-Boltzmann distribution but has a similar shape. There are large numbers of particles at the average energy than at the high and low energy levels. This is due to some of the particles which are not colliding with any other particles and their energy is not changed from its average energy which is assigned in the beginning.

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Chapter 4

Future work

4.1 Introduction

Ideal gas simulation was a foundation for writing simulation codes in C++ for phonon transport. Phonon's properties are different from those of an ideal gas particle, their momentum and energy conservation is governed by different laws. There are different types of phonon interactions unlike only one interaction in an ideal gas. There are also two types of phonons as mentioned in earlier chapters, but we neglect optical phonons as their effect on thermal transport is negligible. Unlike in ideal gas simulation the number of phonons in a given volume is constant. They also have different polarisation. A phonon is either assigned a longitudinal acoustic(LA) branch or a transverse acoustic(TA) branch depending on the Bose-Einstein distribution. The phonons when they interact can either merge to become a single phonon or a single phonon might scatter into two other phonons. Thus future work can be divided into three categories.

a) implementation of phonons in the existing ideal gas molecular dynamics simulation.

b) phonon simulation applied to heterogeneous bulk materials like GaAs, AlGaAs, InGaAs and GaN.

c) phonon simulation applied to devices such as MOSFET, HEMT and SOIFET

4.2 Molecular Dynamic Simulation of Phonons

The details of the phonons properties that are to be considered and the scattering mechanisms are discuscussed in this section of the report.

Initial volume of the block that is considered in the ideal gas simulation remains the same. The number of phonons in the block can not be randomly assigned as in ideal gas simulation, they are governed by the equation 4.1, but we get a very large number of phonons using this equation which is difficult to consider for molecular dynamic simulation. This number can be scaled down to a suitable number for our simulation.

$$N(p) = \sum_{i=1}^{N_b} \langle n(\omega_{o,i}, p) \rangle D(\omega_{o,i}, p) \Delta\omega_i \tag{4.1}$$

The positions of the phonons are assigned randomly in the block similar to ideal gas simulation. The velocity will be the group velocity given by the equation 4.2 [1, 19].

$$\mathbf{V}_g = \nabla_k \omega \tag{4.2}$$

The frequency of the phonon is determined using the dispersion relationship of the material. The maximum cut off frequencies of LA and TA are found from the dispersion curve. The frequency space between ω_{maxLA} is divided into N different spectral intervals. A random number is drawn which is within the spectral interval. The frequency of the phonon can be given by the equation 4.3

$$\omega = \omega_{0,i} + (2R - 1)\frac{\Delta\omega_i}{2} \tag{4.3}$$

4.3   Polarisation

To determine whether a phonon belongs to LA or TA branch the Bose-Einstein distribution is used. A random number is drawn between zero and unity; if the random number is less than $P_i(LA/TA)$ then the phonon belongs to LA branch, otherwise it belongs to TA branch.

4.4   Scattering

Phonons engage is three-phonon elastic interacting of two types: Normal scattering and Umklapp scattering process [1]. The energy conservation for both the types of scattering is given by the equation 4.4

$$\omega1 + \omega2 \leftrightarrow \omega3 \tag{4.4}$$

The momentum conservation for normal scattering is given by the equation 4.5.

$$\mathbf{K}_1 + \mathbf{K}_2 \leftrightarrow \mathbf{K}_3 \tag{4.5}$$

The momentum conservation for Umklapp scattering is given by the equation 2.18.

When both the momentum and energy are conserved only certain types of scattering between the polarisation branches is possible: $LA \Leftrightarrow LA + TA$ and $LA \Leftrightarrow TA + TA$ [20, 21]

This part of work is the most challenging to implement in molecular dynamics using a hard sphere modell. In ideal gas if two particles scatter they remain two particles even after the collision but in the case of phonons two phonons scatter to become one. Exact method to implement this process has to be researched.

4.5 Phonon Simulation Applied to Heterogeneous Bulk Material

In reality the materials used for semiconductor devices are not homogeneous, they are doped with other materials. Taking the phonon molecular dynamic simulation to the heterogenous bulk material is another challenging work. In the heterogeneous material the major constituent can be considered as the main material and the other as a defect in the crystal when the simulations are carried out. When the phonons encounter these defects, the scattering mechanism will be different form the normal or Umklapp scattering. Momentum and energy conservation for this kind of scattering has to be researched. Other problems in heterogeneous materials have to be explored and solved.

4.6 Phonon Simulation Applied to Devices

The devices will have many interfaces between different materials. The molecular dynamics simulation of phonons in these devices will be the most challenging task. The interface between two different materials will lead to different densities and different sound speeds resulting in an acoustic impedance mismatch. This acoustic impedance mismatch will have an effect on phonon transmission. This effect needs to be considered in momentum and energy conservation laws for molecular dynamic simulation of phonons

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