CHAPTER – 6

Self and Impurity Diffusion in Si – Simulation by Chandrasekhar Hopping

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Abstract

The understanding of diffusion is essential to estimate the proper doping levels of impurities in the design of optoelectronic devices and other properties.

The diffusion in silicon is studied, in the present investigation, by simulation using Chandrasekhar hopping. The method employed by Chandrasekhar on the astronomical bodies is applied to study the self and impurity diffusion in silicon. The Fokker-Planck form of the Fick’s law and a smooth continuous position probability density for the diffusing particle $\omega(r,t)$, representing the position of the diffusing particle at any time $t$, is used for the evaluation of the diffusion constant. The results agree reasonably well with the available experimental and other theoretically reported values.
6.1 Introduction

Diffusion, though an old topic, is still being studied in bulk materials and super lattices to understand the mode of transport, because of the various technological applications, particularly in semiconductors. The use of diffusion in the post growth fine tuning of devices based on semiconductor microstructures has become increasingly important. For instance, diffusion of an alloy component $Al$ in $GaAs$, $Mn$ in $CdTe$ or $S$ in $ZnSe$ will affect the opto-electronic properties of the device and could ultimately render the device useless. Hence, both device fabrication and device stability demands quantitative knowledge of the diffusion for the effective controlling of the process.

Computer simulations provide a means of dealing with problems of such complexity that are intractable by analytical and numerical approaches. Even though lattice dynamical investigations on the diffusion process are useful, simulation makes the study simpler. At the same time, the results of such simulations can sometimes reveal features that can lead to successful analytic formulation of a problem. Extensive simulation methods, both Monte Carlo and molecular dynamics are already available [1,2] in the literature. Similarly simulation of diffusion in Si and Ge are also available [3,4], however, the simulation based on Chandrasekhar hopping is presented in this chapter.
Recently, Collins et al. [5] have reported one dimensional diffusion based on unbiased hopping. Chandrasekhar [6] has discussed in detail the stochastic nature of astronomical activities by hopping when he originally worked out the diffusion of the flux tubes from the solar corona on the ionosphere. Similarly the distribution of the temperatures on the photosphere had also been investigated by this approach. The dimensions that are involved in the solar activity are of the order of light years and the temperatures \( \sim 5000^\circ \text{C} \). Such a theory is suitably modified in the present study of atomic diffusion in Si and Ge, where the dimensions are of the order of Å and at ambient temperatures.

Diffusion can also be treated as a stochastic process, since it depends on many parameters like temperature, activation energy, mass of the diffusing particle, lattice parameter, etc., and is described by a probability distribution [7]. Hence, an attempt is made to employ the simulation involving Chandrasekhar hopping for diffusion in real crystal lattices, particularly on Si and Ge, by modifying the model of Collins et al. [5].

### 6.2 Chandrasekhar hopping

Simulation studies on diffusion is not new and plenty of papers are reported in literature on the diffusion in semiconducting systems, based on different models and a good review can be found in Refs. 1 and 2. However, simulation by Chandrasekhar hopping is rarely reported for semiconducting
systems. Detailed theory has been discussed in Ref.[6] and then to some extent in Ref.[5]. For continuity, a brief review is presented here.

To start with, a three dimensional lattice obeying *ding-dong* model is considered, i.e., a modified three dimensional *ding-a-ling* model, is considered [8,9]. The *ding-a-ling* model is a one dimensional chain consisting of the fixed equidistant hard point particles (harmonic oscillators) with equal mass and there is a free particle in between two fixed particles; but in the *ding-dong* model, the fixed harmonic oscillators are allowed to collide and there is no free hard point particle in between.

The length or thickness of the sample of one-dimensional lattice is $L$ along the $x$–axis. It is divided into $N+1$ planes normal to the $x$–axis at an equal spacing of

$$ h = \frac{L}{N} \quad (6.1) $$

Now the $k^{th}$ plane is at a distance $x_k$ (Figure 6.1)

$$ x_k = kh = k \frac{L}{N} \quad (6.2) $$

When the motion of the particles obeys Chandrasekhar type behaviour, then the hopping statistics of the particle from plane $k$ depends only on that plane and is independent of the previous history of the particle.

Now the particle is allowed to hop from plane $k$ either to plane $k-1$ or $k+1$ with equal probability, say $\frac{1}{2}$. The mean hop rate for a particle from plane $k$ is $v_k$ which varies from site to site but maintains symmetric scattering at any
Fig. 6.1. One-dimensional lattice of length $L$, with $N$ equally spaced planes.
one site. The spatial dependence of diffusion arises from the variation in $v_k$ from site to site. So in an ensemble of such particles with a hop rate $v_k$, the mean dwell time on plane $k$ is of the order of $v_k^{-1}$.

Let the particle be in an arbitrary interior plane $k$ at time $t = 0$. Let $W_k(t)$ be the probability that the particle is on plane $k$. Then the time-dependent equation for the interior planes is given as

$$\frac{dW_k}{dt} = \frac{1}{2} v_{k-1} W_{k-1} - v_k W_k + \frac{1}{2} v_{k+1} W_{k+1} \quad (2 < k < N-1) \quad (6.3)$$

The positive terms represent the transfer of particles from planes $k-1$ and $k+1$ to $k$ and the negative term represents the transfer from plane $k$ to $k-1$ and $k+1$. The end planes $k = 0$ at $x = 0$ and $k = N$ at $x = L$ are either both reflecting or absorbing. The particle would be found on any one of the planes $0, 1, 2, 3 ... N$ at any time. Therefore

$$\sum_{k=0}^{N} W_k = 1 \quad (6.4)$$

If the diffusion equation is considered to represent the hopping process in such cases, then the continuous probability density is given by

$$\omega(x_k, t) = \frac{W_k(t)}{h} = \frac{NW_k(t)}{L} \quad (6.5)$$

i.e., the plane probability is divided by the distance between the planes.
The continuous smoothed probability density \( \omega(x,t) \), which is a smooth interpolation of the \( \omega(x_k,t) \) at the site planes, is then related to the current density \( J \) through the particle conservation relation

\[
\frac{\partial \omega(x,t)}{\partial t} = -\frac{\partial J}{\partial x}
\]  

(6.6)

Then the generalized Fick's law for diffusion in the case, where diffusivity \( D \) is position dependent, as discussed by Van Kampen [10], Landauer [11], and Landsberg [12], is considered

\[
J = -\frac{\partial}{\partial x} [D(x)\omega(x,t)]
\]  

(6.7)

This is in the spirit of the Fokker-Plank equation, as given by Risken [13]. If the momentum distribution attains local equilibrium much more rapidly than the coordinate distribution and described by a Boltzmann distribution, the spatial distribution \( \omega(x,t) \) may be reduced to a diffusion equation, from eqn.(6.7) to

\[
\frac{\partial \omega(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2} [D(x)\omega(x,t)]
\]  

(6.8)

It is known that in Chandrasekhar random flights model, if the hopping is locally symmetric and the boundaries are absorbing then the probability density \( \omega(r,t) \) satisfies the sum rule

\[
\langle r(t) \rangle = \int \omega(r,t) d^3r = r_i \quad \text{for all } t > 0
\]  

(6.9)
where \( r_i \) is the initial position of the particle and the integral is taken over all space accessible to the particle. In discrete form the relation reduces to

\[
\langle r(t) \rangle = \sum_{k=0}^{N} kW_k = i
\]  

(6.10)

where \( i \) is the initial plane location.

Although the distribution is symmetrical at \( t=0 \) and in the limit \( t \to \infty \), it can be seen from Fig.6.2, that the symmetry is destroyed at all intermediate times, there being a pronounced shift in the probabilities towards the low temperature region. In this case, the sum rule takes the form

\[
\sum_{k=0}^{N} kW_k = \frac{N}{2}
\]  

(6.11)

In the case of reflecting end planes the sum rule does not apply and the shift in the probability towards the low temperature side is not compensated by absorption probabilities, tending towards the limiting distribution with probabilities,

\[
W_k^* = \frac{\frac{1}{V_k}}{\sum_{k=0}^{N} \left( \frac{1}{V_k} \right)}
\]  

(6.12)

The corresponding asymptotic value \( \langle x \rangle^* \) of the expectation value of the particle position \( \langle x(t) \rangle \) is given by
Fig. 6.2. Probability profiles. (Central Peak value scaled down)
X-axis indicates the position of the atomic planes in arbitrary units
and Y-axis shows the probability (un-normalized) values.
The peak of the curve
(a) represents the initial position of the diffusing atom (time t=0)
(b), (c) and (d) represent the first, second, and third jumping
positions of the atom respectively
and the other curves represent the succeeding jumps of the
diffusing atom.
There are two cases of diffusion in the Chandrasekhar random-flights model.

(1) In the first case, the end planes of the system would be absorbing, i.e., the diffusing particles would reach the end planes.

(2) In the second case, the end planes are reflecting, i.e., the particles are reflected back into the system.

This implies that the diffusing particles will tend to be \textit{trapped} in regions of low jump rate as time evolves with a resulting enhancement of probability density in the colder region.

\section*{6.3 Simulation}

The present simulation does not involve the well known Metropolis and Verlett algorithms that are necessarily to be followed for diffusion related Monte Carlo and Molecular Dynamics simulation problems. Let us consider a cubic lattice of side \(L\), divided into \(N\) equally spaced parts (say, \(h=L/N\), along all the three axes. Every dividing point along the axes is then considered to be the positions of the atoms on the lattice and \(h\) is the lattice parameter (which is usually referred to as \(a\)).
Let the ensemble on one side consists of \( N \) atomic sites, equally spaced by distance of the lattice parameter \( a \). Then the total length of the ensemble on that side can be expressed as

\[
L = Na
\]  

(6.14)

Now we apply a linear temperature gradient along that side of the sample by keeping one end \((r=0)\) at a temperature \( T_0 \), known as ‘cold end’ and the other end \((r=L)\) at a higher temperature \( T_L \), known as ‘hot end’. Now \( T(r) \) is given approximately as

\[
T(r) = T_0 + (T_L - T_0) \frac{r}{L} \quad (0 \leq r \leq L)
\]  

(6.15)

It is known that

\[
h \nu_0 = k_B \theta_D
\]  

(6.16)

where \( h \) is the Planck’s constant, \( k_B \) is the Boltzmann constant, \( \nu_0 \) is the Debye frequency and \( \theta_D \) the Debye temperature.

It is also known that

\[
\Gamma = \Gamma_0 \exp \left( \frac{-\Delta E}{k_B T} \right)
\]  

(6.17)

from diffusion theory, where \( \Gamma_0 \) and \( \Gamma \) are the attempt and jump frequencies. In general the attempt frequency \( \Gamma_0 \) will be of the order of Debye frequency \( \nu_0 \), from experience on other systems. Following this, the position dependent jumping frequency can be written as
\[ v(r) = v_0 \exp\left(\frac{-\Delta E}{k_B T(r)}\right) \tag{6.18} \]

where \( \Delta E \) is the activation energy at the saddle point, which has a spatial dependence.

If a finite life time (dwelling time) is associated with the occupation of a given lattice site by a particular atom, then the mean dwelling time of the particle on a particular site shall be approximated by the relation

\[ t = \frac{1}{v(r)} \tag{6.19} \]

In real crystal lattices the surrounding atoms across the saddle points will restrict the movement of the diffusing atom. The duration of the diffusion or the hopping process from one site to another will face all such effects. This is represented by a dimensionless parameter,

\[ \tau = C \frac{tD_c}{L^2} \tag{6.20} \]

where \( C \) is a constant, whose magnitude will also have effects due to the correlation and

\[ D_c = \frac{1}{2} v_0 a^2. \tag{6.21} \]

Before hopping, the atom actually fluctuates for some time, during which it receives the necessary energy from the surrounding atoms, which is known as the Short-lived Large Energy Fluctuations of atomic particles (SLEF) \[14\] formation time \( (\tau_1) \). During hopping some energy is spent and
after hopping, the remaining energy is given back to the surrounding atoms, which is known as the SLEF relaxation time \( (\tau_2) \). The magnitudes of the SLEF formation time and relaxation time are almost equal. The duration of the hopping event is actually the sum of these two durations, \( (\tau = \tau_1 + \tau_2) \)

The position of the jumping atom \( r \) is found out using the probability density \( \omega(r,t) \).

\[
\omega(r,t) = \frac{1}{2L \pi \exp \left( \frac{-\Delta E}{k_BT} \right)^{1/2}} \exp \left\{ \frac{-\left( r - \frac{1}{2} \right)^2}{4L^2 \tau \exp \left( \frac{-\Delta E}{k_BT} \right)} \right\} \quad (6.22)
\]

The probability density profiles are evaluated at every atomic site after every atomic jump. From this, it is found that there is a pronounced shift in the probabilities towards the cold end (left) as can be seen in Fig.6.2. These shifts clearly give us the jump positions of the diffusing atom at different times. From this the local diffusivity \( D(r) \) is evaluated using the equation

\[
D(r) = M \frac{<r^2>}{2nt} \quad (6.23)
\]

where \( M \) is the number of hops the particle makes to the adjacent site before stopping at the end of the diffusion time \( \tau \), \( <r^2> \) is the mean square displacement, \( t \) is the time taken and \( n=1, 2 \& 3 \) for one-, two- and three-dimensional systems respectively.

Then the diffusion constant is obtained from
Do $AE = D(r) \exp \left( \frac{\Delta E}{k_b T} \right)$ (6.24)

In the case of two- and three-dimensional systems, the atoms can jump in more than one direction. Therefore, in realistic systems of Si, Ge, etc., a random number is generated to fix the jump direction. The schematic of this process is shown in Figs. 6.3 (a),(b) and (c). In each case the displacement is evaluated and hence the diffusivity.

In the present study of self and Ge diffusion in Si, the lattice parameter ‘\(a\)’, the Debye temperature \(\theta_D\), the activation energy \(\Delta E\) and the temperatures at both ends of the specimen \(T_0\) and \(T_L\) are fed as input to execute the simulation program, that is developed.

6.4 Traps

Now, the probability profiles as seen in Fig. 6.2 indicate the jumping of atom, towards the (left) lower temperature region. When the boundaries are reflecting, the displacements of the successive jumps tend to decrease and at some stage the atom stops jumping as indicated in Figs. 6.3 (a) and (b). When this happens, the atoms are said to be trapped at such sites and these potential traps are normally distributed in regions of low temperature gradient. These potential traps could be crystalline defects, agglomerates of the diffusing atoms, same type of atoms with a tendency to form a molecule or impurity atoms whether they be dopant ions or contaminating impurities. Rapid interstitial migration of the atomic species may also occur due to the presence
Fig.6.3(a). Path of the Si atom in Si, when the end planes are reflecting (in 2D)
I – Initial position of the diffusing atom, $T_p$ – position of the trap, where the particle is trapped, a, b and c are the intermediate positions of the jumping atom. X and Y-axes indicate the x and y coordinates of the positions of the jumping atom.
Fig. 6.3(b). Path of the Ge atom in Si, when the end planes are reflecting (in 2D)
I – Initial position of the diffusing atom, $T_p$ – position of the trap, where the particle is trapped, $a$, $b$, and $c$ are the intermediate positions of the jumping atom. $X$ and $Y$-axes indicate the $x$ and $y$ coordinates of the positions of the jumping atom.
Fig. 6.3(c). Path of the Si atom in Si, when the end planes are absorbing (in 2D)
I – Initial position of the diffusing atom, A – position at the cold end plane, where the particle is absorbed, a, b and c are the intermediate positions of the jumping atom. X and Y-axes indicate the x and y coordinates of the positions of the jumping atom.
of the trapping sites. Pearton et al [15] have worked out the diffusivity of hydrogen in crystalline semiconductors and explained the influence of the traps on the diffusivity.

The presence of traps reduces the apparent diffusivity leading to an effective diffusion coefficient. Wert et al [16] have shown that the apparent diffusion coefficient falls off rapidly with a sub linear dependence at low temperatures as a function of either trap concentration or trap binding energy. Rahbi et al [17] and Seager et al [18] have also reported the effect of traps in their work on diffusion. Mathiot [19] in his model for diffusion in n-type and p-type Si, explicitly introduces a term to account for the trapping of the diffusing particle at unidentified traps.

The present simple model, clearly demonstrates the presence of the potential traps in the low temperature region even when explicit terms are not included in the model for traps, viz, Chandrasekhar type hopping mechanism for diffusion is certainly capable of demonstrating the presence of traps in the crystalline media.

6.5 Results and Discussion

The present model does not consider in detail the microscopic mechanical behaviour of the particles involved, such as their trajectories, potential surfaces, saddle points etc. Instead, the model describes statistically the kinetics of the correlated short term motion of the hopping atom and many surrounding atoms during the diffusion process of duration $\tau$. 
A lattice consisting of $10^6$ atomic sites along one side is considered and the diffusing particle is placed at the middle of the lattice. Fig. 6.2 illustrates clearly the shifting of the probability profiles towards the cold end, indicating that the diffusing particle is hopping from the hot region to the cold region. It is to be noted that the profile at the centre has a sharp and symmetric peak, confirming the presence of the particle at the initial position towards the centre of the sample. As time increases, the curve shifts towards the low temperature region and also the symmetry is destroyed at all other intermediate instances of time.

For the sake of simplicity, a case of two dimensional lattice is considered. The path of the diffusing particle in a two dimensional lattice is shown in Figs. 6.3 (a), (b) and (c). A very important observation emerging from this study is that the diffusing particles are found trapped at positions nearer the cold end, marked as $T_p$ in Figs. 6.3 (a) and (b), when the temperature of the cold end $T_0$ is kept at temperatures below the Debye temperature ($\Theta_D = 645$ K for Si). It is evident from Figs. 6.3 (a), (b) and (c) that the trap is formed only when the cold end temperature is kept below 645 K in the case of Si. Now the boundaries are said to be reflecting. For example, for Si self diffusion in a lattice consisting of $10^6$ planes, each plane being separated by a lattice constant and when the end planes are reflecting, a particle placed at the position corresponding to the midway between the planes along the x-axis and at a point 25 planes away along the y-axis, which is at

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a temperature of 1550 K, hops to various positions and finally gets trapped at
the position $T_p$, which is at a temperature of 569.79 K as seen in Fig. 6.3(a). In
this case the cold end temperature is 500 K, which is less than the Debye
temperature of Si (645 K). When the cold end temperature is increased above
the Debye temperature, the boundaries become *absorbing* and the particle
simply hops to the boundary (colder) and gets absorbed, as in Fig. 6.3(c),
where the cold end temperature is 675 K.

Ulf Söderval [3] has suggested that the temperature dependence of the
isotope effect can identify the migration process. All his experimental
measurements of isotope effect on boron, gallium and germanium in silicon,
suggest that there is a change from one to another mechanism of diffusion at $\sim$
1050°C in silicon. This supports the result of Hettich *et al* [20] that below
1050°C diffusion is through vacancy only and above 1050°C this is due to
kick out mechanism. Buda *et al* [21] have reported an *ab initio* molecular
dynamics simulation of high temperature proton diffusion in crystalline Si and
found that the diffusion proceeded via a jump-like mechanism.

The Arrhenius plots for the diffusion in Si from the present work are
given in Figs. 6.4 (a) and (b). Different slopes are found in different regions,
while in general, only a single slope is expected. Such observations are
reported by Redington [22], where Arrhenius plot with two straight parts of
different slopes, separated by a knee for Ba self diffusion in BaO. The results
indicate that in the low temperature regime, atoms migrate by coherent
Fig. 6.4(a). Arrhenius plot for self-diffusion in Si.
Fig. 6.4(b). Arrhenius plot for Ge diffusion in Si.
tunnelling resulting in a low diffusivity rate and at high temperatures, the diffusion takes place at a faster rate. The possible reasons for this could be the thermally activated tunnelling to excited state transitions, the thermally excited over-the-barrier jumps and the fluid like motion [23].

It is clear from the Figs. 6.4 (a) and (b) that three different slopes are observed in the temperature regions (i) 1650 K to 1125 K, (ii) 1125 K to 850 K and (iii) 850 K to 650 K. Therefore, three different types of mechanisms with different activation energies may be possible for the diffusing atoms. Thus, the results agree very well with the results of Hettich et al [20]. But in the case of Ge diffusion in Si, the first and second parts of the Arrhenius plot between temperatures 1600 K to 1150 K and 1150 K to 900 K have almost the same slope. Therefore, in this case the same mechanism of diffusion may be active in both the regions. But the third region between temperatures 900 K to 750 K has a different slope. The dominant mechanism of diffusion requires lowest activation energy. The exact mechanism is not determined in this method and further work can be done to analyse the diffusion mechanisms also using the Chandrasekhar hopping, even though the present results establish the fact that different diffusion mechanisms are active in different temperature regions, in Si.

The pre factors evaluated by the present simulation are given in Tables 6.1 and 6.2 and also shown in Figs. 6.5 (a) and (b) along with the experimental results and the previously reported theoretical values [24]. The agreement
Table 6.1. Comparison of diffusivity (pre factor $D_0$) with the experimental and theoretical data for Self-diffusion in Si.

<table>
<thead>
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<td>1.43</td>
<td>2.04</td>
<td>750- 850</td>
</tr>
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<td>4.10</td>
<td>0.90</td>
<td>0.70</td>
<td>0.86</td>
<td>-----</td>
<td>650- 750</td>
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Table 6.2. Comparison of diffusivity (pre factor $D_0$) with the experimental and theoretical data for Ge-diffusion in Si.

<table>
<thead>
<tr>
<th>$\Delta E$ (eV)</th>
<th>$\ln D_0$ Experiment [24]</th>
<th>$\ln D_0$ Theory [24]</th>
<th>$\ln D_0$ Present work</th>
<th>Temp.range $K$</th>
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<td>5.355</td>
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<td>4.39</td>
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<td>3.28</td>
<td>3.23</td>
<td>900-1150</td>
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<td>4.700</td>
<td>3.18</td>
<td>2.50</td>
<td>2.51</td>
<td>750-900</td>
</tr>
</tbody>
</table>
Fig. 6.5(a). The pre factor $D_0$ (Diffusivity) for various values of activation energy in Si self-diffusion.
Fig. 6.5(b). The pre factor $D_0$ (Diffusivity) for various values of activation energy in Ge diffusion in Si.
between them is quite good, indicating that the simulation by Chandrasekhar-hopping model works well like any the other established procedures on diffusion.

Uma Maheswari [25] has studied the Si self diffusion employing Monte Carlo simulation, by random walk technique with a simulation cell of 12×12×12. A single vacancy has been assumed for diffusion even though interstitial and substitutional defects are possible. The diffusion has been achieved through jumps. But all the jumps are not successful because of the barrier potential and the interaction of the neighbours. This is incorporated through Metropolis algorithm, without considering many of the crystal properties. Lattice constant for Si is the only parameter that has been used. The pre factor \(D_0\) has been calculated from the slope \((2D_0t)\) of the graph \(\log C vs x^2\), where \(C\) is the concentration and \(x\) is the displacement and this has been repeated for various temperatures. The results obtained from this simulation agree reasonably well with the experimental as well as other theoretical [24] results. Impurity (arsenic) diffusion in Si has also been studied, since experimental results are available for As diffusion in Si and encouraging results have been obtained. But this simple simulation has many drawbacks, as mentioned earlier, i.e., none of the actual physical and crystalline properties of Si or As has been considered except the mass changes. Still, within the limit of the calculations the agreement with the experiment is quite good. However, the presence of traps could not be established.
But, in the present work employing Chandrasekhar hopping, a new technique of simulation is achieved, where in all the properties of Si are included through Debye temperature and the interesting properties of diffusion, including the presence of traps, are deduced.

A FORTRAN source code has been developed exclusively to obtain the diffusion profile. A single run of this program on a PC (800 MHz) took about 30 minutes for execution. This program has to be executed for different temperatures and different initial positions, to study the nature of diffusion.

6.6 Conclusion

Diffusion studies in Si and Ge, for both self and impurity, by experiment and theory are available in literature and of late by simulations. Even though many of the investigations employ either Monte Carlo or Molecular Dynamics simulation, a relatively new approach for diffusion is presented. The method used for astronomical activities is extended to study the self and impurity diffusion in Si i.e., at microscopic level. Collins et al [5] had worked out a one dimensional problem to demonstrate the Chandrasekhar hopping. This model is extended to study the self and impurity diffusion in real three dimensional Si crystal with suitable modifications. The results obtained from the present simulation, as shown in Figs. 6.5 (a) and (b), agree well with the experimental results and the previously reported theoretical values [24].
Thus, the Chandrasekhar hopping, though developed originally in astronomy, can be extended to microscopic level such as crystalline systems. Various ising models, including Monte Carlo and Molecular dynamics simulations can be refined according to Chandrasekhar hopping, to simplify the problem.

Though the exact mechanism of diffusion is not determined, it could be demonstrated that there is a change in diffusion mechanism above and below certain temperatures from the Arrhenius plot (where different slopes are observed in different temperature regions) as seen in Figs. 6.4 (a) and (b). This is an important result from the present simulation work and explains the reasons for two diffusion experiments on the same system giving different results.

Similarly traps and the saddle points are inevitable in the diffusion process. Monte Carlo and Molecular dynamics simulation on the diffusion could not exactly identify the traps. Lattice dynamical investigations treat these traps as singular points in the evaluation of jump frequency and so they will not be explicitly seen in the jumping process. But, in the present model traps could be clearly established, thereby demonstrating that the simulation technique is a more powerful tool in identifying the traps. This observation on different systems can help researchers and industrialists for a flawless study or the fabrication of useful solid state devices.
Similarly the role of anharmonicity in the diffusion process, as higher temperatures are considered, is not completely neglected as many lattice dynamical calculations assume. For example, in the ding-a-ling model, the harmonic oscillators are allowed to collide, which is equivalent to phonon-phonon interactions in crystal physics and is essentially due to anharmonicity.
6.7 References


