Conclusions and Future Scope

7.1 Conclusions

In this concluding chapter, we round up the highlight of results obtained in the previous chapters. Chapter 1 and 3 being a general review of Green’s function and CNTs respectively are excluded.

From chapter 2, we have the following results:

1. The relaxation rate due to defect anharmonic interaction has been found to be given by

\[ \Gamma(qs, \omega) = B\omega^3 T \] (7.1)

where

\[ B = -\frac{\pi^8 \alpha a_0^5 A k_B (\Delta M)}{2\sqrt{3}hM^2 v_c G} \] (7.2)

2. From the above expression (7.1), we find that this relaxation rate has the same temperature dependence as the relaxation rate of three-phonon process which gives a predominant contribution to thermal conductivity at
high temperatures.

3. So, the above relaxation rate (7.1) may contribute significantly to lattice thermal conductivity.

In chapter 4, we study the three-phonon interaction process in semiconducting single-walled carbon nanotubes and obtain the following results:

1. In a semiconducting SWCNT, the relaxation rates (Γ) for the various three-phonon scattering processes are given in Table 7.1 below:

<table>
<thead>
<tr>
<th>Scattering Process</th>
<th>Γ in s(^{-1})</th>
<th>Thermal conductivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>(L \rightarrow F + F)</td>
<td>(\sim 10^{10})</td>
<td>linear increase with increasing temperature</td>
</tr>
<tr>
<td>(T \rightarrow F + F)</td>
<td>(\sim 10^7 - 10^8)</td>
<td>linear increase with increasing temperature</td>
</tr>
<tr>
<td>(B \rightarrow F + F)</td>
<td>(\sim 10^8 - 10^9)</td>
<td>nearly constant at very low temperatures and then increases linearly with increasing temperature</td>
</tr>
</tbody>
</table>

Table 7.1: Relaxation rates for different three-phonon scattering processes.

2. The relaxation rates of these three-phonon scattering processes decrease with increasing radius of the SWCNTs.

3. The thermal conductivity increases with increasing radii of the tubes.

4. The thermal conductivity increases with increasing temperature in the low temperature region and after reaching a peak at around 200 K again decreases with further rise in temperature with the peak position shifting to lower temperatures for larger radii tubes.

5. The optical breathing mode phonons has to be included in evaluating the thermal conductivity to avoid overestimation in thermal conductivity.

From chapter 5, we arrive at the following result
1. The relaxation rate of the four-phonon process is \( \sim 10^{-3}s^{-1} \).

2. The thermal conductivity of four-phonon process (\( \sim 10^{-3} - 10^{-2} \text{ W/mK} \)) gives a relatively small value compared to three-phonon process (\( \sim 10^{2} \text{ W/mK} \)).

3. Thus, three-phonon process having larger transition probability is dominating four-phonon process in thermal conduction.

Lastly, in chapter 6, we conclude that

1. The relaxation rate of second-order resonant three-phonon process is \( \sim 10^{7} - 10^{8}s^{-1} \) and that of the second-order resonant four-phonon process is \( \sim 10^{-4} - 10^{-3}s^{-1} \).

2. Resonant three-phonon and four-phonon processes give lesser thermal conductivities than those given by three-phonon processes.

3. Although resonant three-phonon process has high transition probability, it gives much lesser contribution to thermal conductivity than three-phonon process. This may be due to the fact that the flexural acoustic modes are the lowest-lying mode and hence they transport less energy.

Thus, for a semiconducting SWCNT three-phonon process is the main scattering mechanism contributing largely to thermal conductivity.

7.2 Future scope

The present work is mainly concentrated in studying the thermal transport coefficients of semiconducting SWCNTs. This work can be further extended to metallic SWCNTs and MWCNTs. Also, the technique can be extended to the
calculation of thermal conductivities due to defects in SWCNTs on the assumption that the defect Hamiltonian is small. There may also be cases where this Hamiltonian is not small in which case Perturbation theory cannot be used. We have to look for an alternative method.
Publications and Seminars

List of Publications:


Seminar/Conference/Lecture Series attended:

1. Participated the VIth National Conference of PANE held at the Department of Physics, Tripura University, Suryamaninagar-799130 from 3-4th April 2009 with paper entitled “Relaxation rate of a phonon due to defect-anharmonic interaction”.

2. Attended the “RRI School on Non-Equilibrium Statistical Physics” held between March 22 to April 3, 2010 at Raman Research Institute, Bangalore.

3. Participated the 7th National Conference of PANE held at the Department of Physics, Manipur University, Canchipur-795003 from
Publications and Seminars

5th - 6th October 2010 with paper entitled “Kubo’s formula for thermal conductivity”.


5. Participated the “Workshop on Mathematica” organized by the Department of Mathematics, Manipur University from 7-21 September, 2011.


8. Participated the “UGC-SAP sponsored National Seminar On Recent Trends In Advanced Materials” organised by the Department of Physics, Manipur University on 26th March, 2013.