APPENDIX - I

PHONON FREQUENCY AT THE ZONE-CENTRE

The matrices \( \mathbf{R} \) and \( \mathbf{S} \) are of the order 3 x 3. The secular determinant (Eq. 3.13) easily splits into three (3 x 3) determinant, each one of them resulting in a cubic equation in \( \omega^2 \) of the general form

\[
Z_1 \omega^6 - Z_2 \omega^4 + Z_3 \omega^2 - Z_4 = 0
\]

where

\[
Z_1 = m_A m_B m_C
\]
\[
Z_2 = R(m_B + m_C + m_A) (m_B + m_C) x (1-x) \lambda
\]
\[
= m_A \{m_Bx^2 + m_C (1-x)^2\}
\]
\[
Z_3 = (m_B + m_C) x (1-x) \lambda R^2 + \{(m_C (1-x)^2 + m_Bx^2) (R^2 - SS^*)\}
\]
\[
+ m_Ax (1-x) \{(x (1-x)R^2 + \lambda x^2R^2 + \lambda (1-x)^2 R^2
\]
\[
+ x(1-x) \lambda R^2 + x(1-x)(1-\lambda)RR^2\}
\]
and

\[
Z_4 = x (1-x) \{R^3 (1-x) \lambda x) (x + (1-x) \lambda x
\]
\[
- R^2 R^* x (1-x)(1-\lambda)^2
\]
\[
- SS^* R (1-\lambda x + x - x^2 = \lambda x^2)
\]
\[
+ SS^* R^* (1-x) (1-\lambda)x\}.
\]

At the point (0,0,0) i.e. the zone centre of the Brillouin zone, it can be easily seen from the expression for various elements \( R \) and \( S \) that \( R = R^* \), \( S = S^* \) and \( R = -S \) and therefore, the general cubic equation (i) reduces to the form

\[
\omega^2 (Z_1 \omega^4 - Z_2 \omega^2 + Z'_3) = 0
\]

where

\[
Z'_3 = (m_A + m_B + m_C) x (1-x) \lambda R^2
\]
This gives one of the solutions as
\[ \omega^2 = 0. \]

Corresponding to the acoustical phonons at the zone-centre.

The four zone-centre frequencies for the mixed crystal system \( AB_{1-x}C_x \) for \( 0 < x < 1 \) are now obtained as the roots of the equation (ii) quadratic in \( \omega^2 \).

The two longitudinal phonons (\( LO_1 \) and \( LO_2 \)) are obtained by putting

\[ |R_{xx}(q,1)| \]

and two transverse optical phonons (\( TO_1 \) and \( TO_2 \)) by using

\[ |R_{xx}(q,11)| \]

in equation (ii).

**PHONON FREQUENCIES IN THE (1,0,0) DIRECTION**

In this case, the \((9 \times 9)\) secular determinant splits into three \((3 \times 3)\) determinants, two of them being identical. These when solved result into two cubic equations of general nature given by equation (i). The first cubic equation in \( \omega^2 \) is obtained by putting

\[ |R_{xx}(\tilde{q},11)| \]

and \( |S_{xx}(\tilde{q},12)| \) giving three longitudinal phonons (2 longitudinal optical and 1 longitudinal acoustical). The second cubic equation in \( \omega^2 \) is determined by putting

\[ |R_{xx}(\tilde{q},11)| \]

and \( |S_{xx}(\tilde{q},12)| \).

**PHONON IN (1,1,0) DIRECTION**

We get nine different phonons

1. \[ |R_{xx}(\tilde{q},11)| + |R_{xy}(\tilde{q},11)| \]

and

\[ |S_{xx}(\tilde{q},12)| + |S_{xy}(\tilde{q},12)| \]

give the first set of three longitudinal phonons.
II. \[ |R_{xx}(\tilde{q},11)| - |R_{xy}(\tilde{q},11)| \]

and

\[ |S_{xx}(\tilde{q},12)| - |S_{xy}(\tilde{q},12)| \]

gives the second set of three transverse phonons.

III. \[ |R_{zz}(\tilde{q},11)| \]

and

\[ |S_{zz}(\tilde{q},12)| \]

gives the third set of three transverse phonons.

**PHONONS IN (1,1,1) DIRECTION**

The two of the determinant being identical, only two different cubic equations are obtained

I. \[ |R_{xx}(\tilde{q},11)| + 2|R_{xy}(\tilde{q},11)| \]

and

\[ |S_{xx}(\tilde{q},12)| + 2|S_{xy}(\tilde{q},12)| \]

gives the first set of three longitudinal phonons and

II. \[ |R_{xx}(\tilde{q},11)| - |R_{xy}(\tilde{q},11)| \]

and

\[ |S_{xx}(\tilde{q},12)| - |S_{xy}(\tilde{q},12)| \]

gives the second set of three transverse phonons.
APPENDIX – II

Tables for the variation of the non-randomness parameter $\lambda$ with the concentration $x$ for the III-V ternary mixed systems.

**InP$_{1-x}$ As$_x$**

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.22</th>
<th>0.34</th>
<th>0.56</th>
<th>0.61</th>
<th>0.78</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.66</td>
<td>3.6896</td>
<td>4.3036</td>
<td>4.628</td>
<td>6.6743</td>
</tr>
</tbody>
</table>

**Ga$_{1-x}$ Al$_x$Sb**

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.15</th>
<th>0.45</th>
<th>0.66</th>
<th>0.872</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>6.3644</td>
<td>3.1192</td>
<td>2.85</td>
<td>2.664</td>
</tr>
</tbody>
</table>

**Ga$_{1-x}$ As$_x$**

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.25</th>
<th>0.50</th>
<th>0.75</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>4.25</td>
<td>4.34</td>
<td>3.19</td>
</tr>
</tbody>
</table>

**Ga$_{1-x}$ In$_x$As**

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.30</th>
<th>0.38</th>
<th>0.70</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>5.19</td>
<td>5.38</td>
<td>5.41</td>
</tr>
</tbody>
</table>

**InAs$_x$Sb$_{1-x}$**

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.18</th>
<th>0.75</th>
<th>0.825</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.75</td>
<td>4.25</td>
<td>4.78</td>
</tr>
</tbody>
</table>

It is obvious from the above Table that the variation of $\lambda$ with $x$ is not the same for all the mixed systems studied, as for InP$_{1-x}$ As$_x$ and Ga$_{1-x}$In$_x$As, $\lambda$ is increasing with the increasing values of $x$ and for Ga$_{1-x}$ Al$_x$Sb it is decreasing with $x$, for GaP$_{1-x}$ As$_x$ and InAs$_x$Sb$_{1-x}$ no particular behaviour is observed. Therefore we have not been able to define a function $\lambda$ in general as a function of $x$. 
APPENDIX – III

Tables for the variation of the non-randomness parameter $\lambda$ with the concentration $x$ for the II-VI ternary mixed systems.

$\text{Cd}_x\text{Hg}_{1-x}\text{Te}$

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.13</th>
<th>0.20</th>
<th>0.22</th>
<th>0.28</th>
<th>0.34</th>
<th>0.38</th>
<th>0.54</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>10.96</td>
<td>9.75</td>
<td>9.19</td>
<td>10.57</td>
<td>10.49</td>
<td>10.70</td>
<td>12.71</td>
</tr>
</tbody>
</table>

$\text{Mn}_x\text{Hg}_{1-x}\text{Te}$

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.35</th>
<th>0.45</th>
<th>0.6</th>
<th>0.69</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>6.378</td>
<td>5.297</td>
<td>5.189</td>
<td>6.04</td>
</tr>
</tbody>
</table>

$\text{Cd}_{1-x}\text{Mn}_x\text{Te}$

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.3</th>
<th>0.5</th>
<th>0.65</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.19</td>
<td>4.75</td>
<td>3.57</td>
</tr>
</tbody>
</table>

$\text{ZnS}_{1-x}\text{Se}_x$

<table>
<thead>
<tr>
<th>$x$</th>
<th>0.2</th>
<th>0.4</th>
<th>0.68</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.9314</td>
<td>4.15</td>
<td>5.9</td>
</tr>
</tbody>
</table>

From these Tables it is clear that for $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$, $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ and $\text{Mn}_x\text{Hg}_{1-x}\text{Te}$ no particular behaviour for the variation of the non-randomness parameter $\lambda$ with the concentration $x$ is observed and for $\text{ZnS}_{1-x}\text{Se}_x$, $\lambda$ is increasing with the increasing values of $x$.

Therefore we could not define the function $\lambda (x)$ analytically as its variation with $x$ is not the same for all mixed systems studied in the present thesis.