Ramji Rao’s method of evaluating Gruneisen parameter from third order elastic constant.

M. Yousuf Hussain Ansari, M. Wahed Hussain, S.Venkateswara Rao and G. Lavanya

Abstract: Thermal expansion is directly related to anharmonicity of atomic vibration. In theory of thermal expansion coefficient of solid must take into account the anharmonic nature of the lattice. Gruneisen considered the frequencies of vibration as volume dependent. His treatment is considered as quasi harmonic approximation. The volume dependence of atomic frequency is real conceptual contribution of Gruneisen. Our basic objective is to evaluate Gruneisen constant using third order elastic constant by Ramji Rao’s method.

I. Introduction

In recent years considerable amount of data has been generated on second and third order elastic constants. Though Burger and Mason developed expressions for mode gammas and average gamma for SOEC and TOEC but their methods have not received sufficient attention. A modified method for evaluation of average gruneisen constant from third order elastic constant proposed by Ramji Rao (1974); this method also has remained practically unexplored.

Ramji Rao Method of Evaluating Gruneisen Constant.

The Anderson Gruneisen parameter \( \gamma \) is defined by the following equations;

\[
\gamma = - \frac{1}{a} \left( \frac{\partial \ln B}{\partial T} \right)_p
\]

\[
\gamma = \frac{\gamma_R}{\gamma_T} - 1
\]

Where B is bulk modulus. Chang (1967) has shown that the Anderson – Gruneisen parameter \( \gamma \) is simply related to the Gruneisen parameter \( \gamma \) as follows;

\[
\gamma = 2\gamma
\]

Using the formalism of Ramji Rao and Srinivasan (1969), Ramji Rao (1974) showed that the Anderson Gruneisen parameter for cubic crystal can be expressed in terms of the second order elastic constant and third order elastic constant as follows:

\[
\gamma = -1 - (1/3) \left[ \frac{\partial \ln B}{\partial \ln p} \right]
\]

In view of equation (3), the Gruneisen constant can be expressed as:

\[
\gamma = - \frac{1}{2} - \frac{1}{6} \left[ \frac{\partial \ln B}{\partial \ln p} \right]
\]

This equation provides an alternative method for the evaluation of Gruneisen constant from SOEC and TOEC we shall call these values \( \gamma_{RR} \).

Ramji Rao applied this method to only one crystal viz. MgO. As TOEC data are available for several cubic compound crystals, we have evaluated the Gruneisen constant for several crystals using Ramji Rao’s method. The input SOEC and TOEC is same as that we have used for Masor Burger method of evaluating Gruneisen constant. For convenience we have included the same data related to SOEC and TOEC in Table (1). The source of Thermal Gruneisen Constant was obtained with the help of following equation.

\[
\gamma = \frac{3\alpha \Psi}{C_v}
\]

where \( \alpha \) is the coefficient of expansion.

\( \Psi \) is the compressibility and \( C_v \) is the specific heat at constant volume.

It is also same as that of Mason Burger method.

DOI: 10.9790/4861-1004023234

www.iosrjournals.org
Ramji Rao’s method of evaluating Gruneisen parameter from third order elastic constant.

The results of calculations are given in the Table (2).

Table (1)

Input data for calculation of $\gamma'$s by Mason – Burger method and Ramji Rao’s method

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
<th>Ref</th>
<th>$C_{111}$</th>
<th>$C_{112}$</th>
<th>$C_{123}$</th>
<th>$C_{144}$</th>
<th>$C_{166}$</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiF</td>
<td>12.46</td>
<td>4.24</td>
<td>6.49</td>
<td>a</td>
<td>-142.0</td>
<td>-26.40</td>
<td>15.86</td>
<td>8.50</td>
<td>-27.30</td>
<td>g</td>
</tr>
<tr>
<td>NaF</td>
<td>9.71</td>
<td>2.43</td>
<td>2.80</td>
<td>a</td>
<td>-148.0</td>
<td>-27.00</td>
<td>28.00</td>
<td>4.60</td>
<td>-11.40</td>
<td>g</td>
</tr>
<tr>
<td>NaCl</td>
<td>3.87</td>
<td>0.97</td>
<td>0.97</td>
<td>a</td>
<td>-84.30</td>
<td>-2.40</td>
<td>4.60</td>
<td>2.90</td>
<td>-6.00</td>
<td>g</td>
</tr>
<tr>
<td>KCl</td>
<td>4.83</td>
<td>0.54</td>
<td>0.66</td>
<td>a</td>
<td>-72.60</td>
<td>-1.80</td>
<td>1.10</td>
<td>2.30</td>
<td>-2.60</td>
<td>g</td>
</tr>
<tr>
<td>RbCl</td>
<td>3.65</td>
<td>0.61</td>
<td>0.48</td>
<td>a</td>
<td>-67.10</td>
<td>-95.00</td>
<td>0.50</td>
<td>1.10</td>
<td>-1.70</td>
<td>g</td>
</tr>
<tr>
<td>MgO</td>
<td>28.60</td>
<td>8.70</td>
<td>14.80</td>
<td>a</td>
<td>-489.50</td>
<td>3.50</td>
<td>11.30</td>
<td>6.60</td>
<td>-69.00</td>
<td>g</td>
</tr>
<tr>
<td>PbTe</td>
<td>10.795</td>
<td>0.764</td>
<td>1.343</td>
<td>b</td>
<td>185.00</td>
<td>-30.80</td>
<td>9.70</td>
<td>4.40</td>
<td>-9.80</td>
<td>g</td>
</tr>
<tr>
<td>GaSb</td>
<td>8.850</td>
<td>4.040</td>
<td>4.33</td>
<td>a</td>
<td>-47.30</td>
<td>-38.70</td>
<td>-4.40</td>
<td>5.00</td>
<td>-21.60</td>
<td>g</td>
</tr>
<tr>
<td>GaAs</td>
<td>11.88</td>
<td>5.38</td>
<td>5.94</td>
<td>a</td>
<td>-62.20</td>
<td>-47.40</td>
<td>-5.70</td>
<td>-0.20</td>
<td>-26.90</td>
<td>g</td>
</tr>
<tr>
<td>GaP</td>
<td>14.12</td>
<td>6.253</td>
<td>7.047</td>
<td>b</td>
<td>-73.70</td>
<td>-40.00</td>
<td>-13.10</td>
<td>-10.70</td>
<td>-23.40</td>
<td>g</td>
</tr>
<tr>
<td>SrF$_2$</td>
<td>12.461</td>
<td>4.46</td>
<td>3.187</td>
<td>d</td>
<td>-82.10</td>
<td>-29.90</td>
<td>-11.10</td>
<td>-9.57</td>
<td>17.50</td>
<td>d</td>
</tr>
<tr>
<td>BaF$_2$</td>
<td>8.948</td>
<td>3.854</td>
<td>2.495</td>
<td>e</td>
<td>-58.40</td>
<td>-32.10</td>
<td>-20.60</td>
<td>12.01</td>
<td>8.90</td>
<td>e</td>
</tr>
</tbody>
</table>

References

a) Anderson (1965)
b) Simon and wang (1971)
c) Altrovitz and Gerlich (1969)
d) Altrovitz and Gerlich (1970)
e) Gerlich (1968)
f) Manasreh and Pederson (1984)
g) Shankar and Bhende (1986)
h) Ramacahndran and Srinivasan (1972)

Detailed references are provided on the last page.
II. Result and Discussions

After the careful observation of the data following observations are made.

i) In Ramji Rao’s method (Equation 5) provides the values of correct order.

ii) By and large, the values obtained from the equation (5) are larger than thermal values of Gruneisen constant.

iii) The difference between the values calculated from equation (5) varies from crystal to crystal but the difference in the two appear to have a typical value for a family of crystals. Thus the difference is about 30% in the crystals with CaF₂ structure, and it is about 60% in crystals with NaCl structure. Whereas the difference is about 100% - 200% in the crystals with ZnS structure.

iv) In case of PbF₂ there is some difference between \( \gamma_{RR} \) and \( \gamma_{thermal} \). the difference between \( \gamma_{RR} \) and \( \gamma_{MB} \) is not as much as that of \( \gamma_{RR} \) and \( \gamma_{thermal} \).

Acknowledgement

The authors are indebted to Prof. D B Sirdeshmukh for the interest he has shown towards the completion of this project. We are also grateful to the Dr Ch Pursotam Reddy (Chirman of Chaitanya Colleges) and Dr. V Venkataiah (Principal of Chitzanya Postgraduate College) for the facilities they have extended to meet our requirements.

References

[1]. Altrovitz s and Gerlich D (1969)
[2]. Phys. Rev. 184, 999
[3]. Altrovitz s and Gerlich D (1970, a)
[5]. Altrovitz s and Gerlich D (1970, B)
[6]. Phys. Rev. B1, 4136
[7]. Anderson O L (1965)
[9]. Chang (1967)
[13]. Ramachandran V and Srinivasan R (1972)
[14]. Solid Stae Commun. 11, 973
[18]. Phy. Rev. 10, 4173
[19]. Simon G and Wang H
[20]. Single Crystal Elastic constant and calculated Aggregate properties
[21]. (MIT Press, London)