HIGH TEMPERATURE STUDY OF ANHARMONIC PROPERTIES OF LANTHANUM SULPHIDE CRYSTAL

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ABSTRACT

For the deformed face centered cubic crystal one can get the Taylor’s series expansion of elastic energy density starting from nearest neighbor distance and hardness parameter utilizing Coulomb and Born Mayer potentials. The knowledge of the higher order elastic constants for a crystal can be used to obtain the anharmonic properties of the crystals by theoretical approach. The Lanthanum Sulphide crystal possesses face centered cubic crystal structure. The theory is developed for obtaining second, third and fourth order elastic constants of Lanthanum Sulphide single crystals up to an elevated temperature and higher order elastic constants of Lanthanum Sulphide single crystals at an elevated temperature are evaluated. The data thus obtained is used to evaluate the first order pressure derivatives of second and third orders elastic constants, second order pressure derivatives of second order elastic constants and partial contractions.

Keywords: Higher order elastic constants, Hardness parameter, Anharmonic Properties.

INTRODUCTION

In recent material science we need values of elastic constants at elevated temperatures. In the last few years studies of anharmonic properties of monovalent compounds have attracted the attention of the physicists since they provide much valuable information regarding crystal structure1-3. Many properties of crystals are thermodynamically linked with specific heat, thermal expansion and Debye temperature and Grüneisen numbers. Many researchers evaluated the anharmonic properties, such as second, third and fourth order elastic constants (SOECs, TOECs and FOECs), first order pressure derivatives (FOPDs) of SOECs and TOECs, second order pressure derivatives (SOPDs) of SOECs of several ionic crystals. Third and fourth order elastic constant are essential to study a number of anharmonic properties of crystals4-6. The thermal contribution to elastic constants is very significant, the experimental data reveal that in going from 0 K to higher temperature, the values of second order elastic constants (SOECs) are changed considerably even for highly ionic solids like LaS7-10. No complete experimental or theoretical efforts have been made so far in obtaining the temperature variation of anharmonic properties of divalent materials possessing different crystal structures at an elevated temperature11. When the elastic energy density for a strain components; The SOECs, TOECs and FOECs deformed crystal is expanded as a power series of strains using Taylor’s series expansion, the coefficients of the quadratic cubic and quartic terms are known as SOECs, TOECs and FOECs. A number of crystal anharmonicities like specific heat at higher temperature, thermal expansion, temperature dependence of acoustic velocities along different directions, acoustic attenuation, Grüneisen parameters are directly related to SOECs and TOECs12-15. The present paper is mainly focused on the study of temperature variation of higher order elastic constants and their pressure derivatives up to an elevated temperature for LaS using Born Mayer and coulomb potential starting from the nearest neighbor distance and hardness parameter. In the absence of any measured data on the elastic properties at higher temperature for this compound, comparison cannot be made.

Theory

The elastic energy density for a crystal of a cubic symmetry in deformed state can be expanded as16:

\[ U_0 = U_2 + U_3 + U_4 \]

\[ = \frac{1}{2} \sigma_{ijkl} a_{ij} a_{kl} + \frac{1}{3} \sigma_{ijklmn} a_{ij} a_{kl} a_{mn} + \frac{1}{4} \sigma_{ijklmnopq} a_{ij} a_{kl} a_{mn} a_{pq} \]  

(1)

Where \( \sigma_{ijkl} \) and \( \sigma_{ijklmnopq} \) are the SOECs, TOECs and FOECs in tensorial form; \( a_{ij} \) are the Lagrangian strain components; The SOECs, TOECs and FOECs

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Throughout this temperature range LaS exhibits FCC crystal structure. Selecting a few data obtained in this study, the values of TOECs at room temperature are given in Tables 2. The FOPDs of TOECs have been evaluated utilizing data of TOECs and SOECs and the results are shown in Table 3. The whole evaluation is based on the assumption that the FCC crystal structure of the material does not change when temperature varies up to their melting point. The value of $r_0$ and $q$ are taken as $2.8116\times10^{-8}$ cm and $0.345\times10^{-8}$ cm.

### RESULTS AND DISCUSSION

One can observed from table 1 that the C$_{11}$ is larger than other Second order elastic constants at room temperature. Among the calculated third order elastic constants of this material, C$_{456}$ is largest in their absolute values and an order of magnitude larger than the SOECs. Magnitude of other C$_{ijkl}$'s are smaller than those of C$_{456}$. For LaS, the values of C$_{111}$, C$_{123}$, C$_{144}$, C$_{166}$ and C$_{456}$ are positive in nature, while C$_{112}$ is negative in nature at room temperature and shows a linear relationship with temperature variation. Among the calculated fourth order elastic constants for LaS in Table 2, C$_{111}$ is the largest in their values at room temperature. Magnitudes of other C$_{ijkl}$'s are smaller than those of C$_{111}$. The values of C$_{1111}$, C$_{1112}$, C$_{4444}$, C$_{1155}$ and C$_{1266}$ are positive in nature, while C$_{1123}$, C$_{1144}$, C$_{4455}$ and C$_{1255}$ are negative in nature and also verify linear relationship with temperature variation. There are three first order pressure derivatives of second order elastic constants and six first order pressure derivatives of third order elastic constants are presented in Table 3. Among the calculated first order pressure derivatives of third order elastic constants for LaS $dC_{111}/dP$ is larger than other ones. The values of $dC_{123}/dP$, $dC_{144}/dP$ and $dC_{166}/dP$ are positive in nature, while $dC_{111}/dP$, $dC_{112}/dP$ and $dC_{456}/dP$ are negative in nature at room temperature. The second order pressure derivatives of second order elastic constants and the values various partial contractions are shown in Table 4. All the variations discussed above are represented graphically in Figs 1-10.
Table 2 - The FOECs of LaS in 10^{12} dyne/cm^2

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>C_{111}</th>
<th>C_{112}</th>
<th>C_{113}</th>
<th>C_{114}4</th>
<th>C_{414}</th>
<th>C_{1155}</th>
<th>C_{1255}</th>
<th>C_{1266}</th>
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<tbody>
<tr>
<td>300</td>
<td>253.59</td>
<td>0.87</td>
<td>9.36</td>
<td>-2.39</td>
<td>-2.64</td>
<td>14.11</td>
<td>11.76</td>
<td>-2.35</td>
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<tr>
<td>500</td>
<td>212.47</td>
<td>-6.87</td>
<td>6.09</td>
<td>-2.43</td>
<td>-2.84</td>
<td>-2.34</td>
<td>14.02</td>
<td>11.26</td>
</tr>
<tr>
<td>700</td>
<td>171.36</td>
<td>-17.62</td>
<td>2.82</td>
<td>-2.46</td>
<td>-3.04</td>
<td>-2.34</td>
<td>13.93</td>
<td>10.77</td>
</tr>
</tbody>
</table>

Table 3 - The FOPDs of SOECs and TOECs of LaS (Dimensionless)

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>dC_{11}/dP</th>
<th>dC_{12}/dP</th>
<th>dC_{13}/dP</th>
<th>dC_{14}/dP</th>
<th>dC_{15}/dP</th>
<th>dC_{16}/dP</th>
<th>dC_{17}/dP</th>
<th>dC_{18}/dP</th>
<th>dC_{19}/dP</th>
<th>dC_{20}/dP</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>-6.20</td>
<td>-1.00</td>
<td>-2.24</td>
<td>-60.41</td>
<td>2.33</td>
<td>0.61</td>
<td>-2.23</td>
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<tr>
<td>400</td>
<td>-6.10</td>
<td>-0.81</td>
<td>-2.23</td>
<td>-50.01</td>
<td>2.30</td>
<td>0.67</td>
<td>-2.04</td>
<td>2.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>-6.00</td>
<td>-0.62</td>
<td>-2.21</td>
<td>-39.93</td>
<td>2.27</td>
<td>0.72</td>
<td>-1.76</td>
<td>2.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>-5.82</td>
<td>-0.25</td>
<td>-2.19</td>
<td>-20.79</td>
<td>2.21</td>
<td>0.82</td>
<td>-1.49</td>
<td>2.27</td>
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<tr>
<td>1000</td>
<td>-5.58</td>
<td>0.26</td>
<td>-2.16</td>
<td>5.30</td>
<td>2.13</td>
<td>0.96</td>
<td>-0.99</td>
<td>2.21</td>
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</table>

Table 4 - The SOPDs of SOECs in 10^{12} cm^2/dyne and Partial Contraction in 10^{13} dyne/cm^2

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>d^2C_{11}/dP^2</th>
<th>d^2C_{12}/dP^2</th>
<th>d^2C_{13}/dP^2</th>
<th>Y_{11}</th>
<th>Y_{12}</th>
<th>Y_{44}</th>
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</thead>
<tbody>
<tr>
<td>300</td>
<td>55.49</td>
<td>-1.45</td>
<td>-0.11</td>
<td>27.10</td>
<td>0.84</td>
<td>3.80</td>
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<tr>
<td>400</td>
<td>51.83</td>
<td>-1.32</td>
<td>-0.66</td>
<td>23.16</td>
<td>-0.26</td>
<td>3.67</td>
</tr>
<tr>
<td>500</td>
<td>48.48</td>
<td>-1.07</td>
<td>-1.19</td>
<td>19.22</td>
<td>-1.37</td>
<td>3.55</td>
</tr>
<tr>
<td>700</td>
<td>42.48</td>
<td>-0.29</td>
<td>-2.14</td>
<td>11.35</td>
<td>-3.59</td>
<td>3.29</td>
</tr>
<tr>
<td>1000</td>
<td>34.84</td>
<td>1.41</td>
<td>-3.31</td>
<td>-0.44</td>
<td>-4.70</td>
<td>2.91</td>
</tr>
</tbody>
</table>

Fig. 1

Fig. 2

Fig. 3

Fig. 4
CONCLUSIONS

The present study shows the validity of the theoretical approach and one can say that a very little variation of pressure derivatives of higher order elastic constant over temperature shows that the crystal can be used for acoustic purposes where high pressure and temperature is required. Since high temperature study is not possible experimentally, the present theoretical approach will be helpful to study these types of crystals at elevated temperatures. This theoretical approach has been successfully applied for mono-valant and di-valant crystals; also it can be used to study tri-valant crystals.

REFERENCES