ANHARMONIC BEHAVIOUR OF LANTHANUM SELENIDE CRYSTAL AT HIGH TEMPERATURES

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ABSTRACT

A theoretical approach to evaluate the temperature variation of second third and fourth order elastic constants (SOECs, TOECs and FOECs) for FCC crystal structure solids is developed on the basis of long range and short range potentials using some basic parameters like nearest-neighbour distance and hardness parameter. This theoretical approach is used to calculate second, third and fourth orders elastic constants (SOEC, TOEC and FOEC) of Lanthanum Selenide single crystals from temperature range 300 K to1000 K. The knowledge of the higher-order elastic constants for a crystal is useful for obtaining the anharmonic properties of the crystals within the limit of the continuum approximation. The Lanthanum Selenide crystal possesses face centered cubic crystal structure. The data of SOECs, TOECs and FOECs are used to obtain the first-order pressure derivatives (FOPDs) of SOECs and TOECs, second-order pressure derivatives (SOPDs) of SOECs and partial contractions. The data of Lanthanum Selenide crystals obtained through different techniques give important and valuable information about the internal structure and inherent properties of materials.

Keywords: Anharmonic Behaviour, Elastic Constants, Lanthanum Compounds

INTRODUCTION

During past few years, many researchers involved in experimental and theoretical work on anharmonic properties of a number of monovalent and divalent crystals. In material science, we require values of anharmonic properties at high 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 structure. Anharmonic properties of divalent crystals are important because they are relate to the various solid-state phenomena such as inter-atomic potentials, equation of state and acoustic spectra. Thermodynamically the inherent properties of crystals strongly related with specific heat, thermal expansion, Debye temperature and Grüneisen numbers. Various measurements have been made on 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 for a number of ionic crystals. Third and fourth order elastic constant are required to study many anharmonic properties of crystals and therefore their precise evaluation play very important role. In past few years, many researchers calculated anharmonic properties of NaCl type crystals [1-6]. Only few of them studied the temperature dependence of above properties. The laboratory data reveal that in going from 0 K to higher temperature, the values of second order elastic constants (SOECs) changed considerably even in case of divalent crystals like LaSe [7-10]. Many experimental and theoretical studies done on the temperature variation of anharmonic properties of divalent crystals having different crystal structures in high temperature range shows very important results. [11].

When for a deformed crystal the elastic energy density expended as a power series of strains with the help of Taylor’s series, the SOECs, TOECs and FOECs obtained as the coefficients of quadratic cubic and quartic terms respectively. Several physical properties and crystal anharmonicities such as thermal expansion, specific heat at higher temperature, temperature variation of acoustic velocity, acoustic wave attenuation, the FOPDs of SOECs and Grüneisen numbers linked directly to SOECs and TOECs.

Present paper focuses on the study of temperature variation of higher order elastic constants and their
pressure derivatives up to 1000 K for LaSe using Born Mayer and coulomb potentials taking the nearest neighbor distance and hardness parameter as basic parameters. Since the experimental data on the elastic properties at higher temperature is not available for LaSe, the comparison of results is not possible.

Theory

The expansion of elastic energy density for a crystal having cubic symmetry is as \([12, 13]\)

\[ U_0 = U_2 + U_3 + U_4 \]

The first part is the strain derivative of internal energy \(U_0\) and known as static elastic constant and the free energy \(U_{\text{vib}}\) and is called vibrational elastic constant. The second part is the strain derivative of the vibrational free energy density \(U_{\text{vib}}\) and is called vibrational elastic constant.

where the expression for \(g\)'s and \(F\)'s for FCC crystals are as:

\[ C_{ijkl} = \text{const.} \]

Expressions for vibrational contribution to the second, third and fourth order elastic constants are as:

\[ C^{\text{vib}}_{111} = g_1 F^2_1 + g_2 F^2_2 + g_3 F^2_3 + g_4 F^2_4; \]
\[ C^{\text{vib}}_{1112} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]
\[ C^{\text{vib}}_{1122} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]
\[ C^{\text{vib}}_{1111} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]
\[ C^{\text{vib}}_{1123} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]
\[ C^{\text{vib}}_{1112} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]
\[ C^{\text{vib}}_{1111} = g_1 F^2_1 + 2 g_2 F_1 F_2 + g_3 F_2^2 + g_4 F_3^2 + g_5 F_4^2; \]

The theory for the calculation of different anharmonic properties of the substances possessing FCC crystal structures given in the preceding section. The TOECs for LaSe evaluated from 300K to 1000K. Throughout this temperature range LaSe exhibits FCC crystal structure and no phase change occur. Various elastic constants and their pressure derivatives for temperature range from 300 K up to 1000 K (upto melting point) into the interval of 50 K are calculated using small C++ programs and selecting few data obtained in the study, the values of SOECs and TOECs are given in Tables 1. The eleven values of FOECs are given in Table 2. The FOPDs of SOECs and FOPDs of TOECs have been evaluated utilizing data of TOECs and SOECs and the results given in Table 3. The SOPDs of SOECs and partial contractions given in Table 4. The temperature variation curves plotted between various elastic constants and their pressure derivatives with temperature shown in Table 1-12. The taken temperature range is from room temperature 300 K up to 1000 K within interval of 50 K. While doing these calculations the input parameters, nearest-neighbor...
distance ($r_0$), the hardness parameter ($q$), Atomic mass of La (M₁) and Atomic mass of Se (M₂) are taken to be $2.9403 \times 10^8$ cm, $0.345 \times 10^8$ cm, 138.90 and 78.96 respectively.

Table 1 - The SOECs and TOECs of LaSe in $10^{11}$ dyne/cm²

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>C₁₁</th>
<th>C₁₂</th>
<th>C₄₄</th>
<th>C₁₁₁</th>
<th>C₁₁₂</th>
<th>C₁₂₃</th>
<th>C₁₄₄</th>
<th>C₁₆₆</th>
<th>C₁₄₆</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>15.89</td>
<td>5.07</td>
<td>5.21</td>
<td>-218.35</td>
<td>-1.03</td>
<td>9.04</td>
<td>8.68</td>
<td>8.73</td>
<td>8.37</td>
</tr>
<tr>
<td>400</td>
<td>16.46</td>
<td>5.03</td>
<td>5.21</td>
<td>-216.98</td>
<td>-3.73</td>
<td>9.26</td>
<td>8.79</td>
<td>8.79</td>
<td>8.37</td>
</tr>
<tr>
<td>500</td>
<td>17.03</td>
<td>5.00</td>
<td>5.22</td>
<td>-215.63</td>
<td>-6.52</td>
<td>9.48</td>
<td>8.89</td>
<td>8.85</td>
<td>8.37</td>
</tr>
<tr>
<td>700</td>
<td>18.20</td>
<td>4.92</td>
<td>5.23</td>
<td>-212.96</td>
<td>-12.21</td>
<td>9.93</td>
<td>9.10</td>
<td>8.96</td>
<td>8.37</td>
</tr>
</tbody>
</table>

Table 2 - The FOECs of LaSe in $10^{12}$ dyne/cm²

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>C₁₁₁₁</th>
<th>C₁₁₁₂</th>
<th>C₁₁₂₂</th>
<th>C₁₂₁₂</th>
<th>C₁₄₄₄</th>
<th>C₁₄₅₆</th>
<th>C₁₄₆₄</th>
<th>C₁₄₅₅</th>
<th>C₁₂₂₅</th>
<th>C₁₂₆₆</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>243.12</td>
<td>-1.62</td>
<td>6.40</td>
<td>-1.98</td>
<td>-2.22</td>
<td>-1.95</td>
<td>11.66</td>
<td>9.65</td>
<td>-1.96</td>
<td>-2.20</td>
</tr>
<tr>
<td>400</td>
<td>221.51</td>
<td>-5.60</td>
<td>-4.60</td>
<td>-1.99</td>
<td>-2.31</td>
<td>-1.95</td>
<td>11.62</td>
<td>9.43</td>
<td>-1.96</td>
<td>-2.28</td>
</tr>
<tr>
<td>500</td>
<td>199.91</td>
<td>-9.57</td>
<td>2.81</td>
<td>-2.00</td>
<td>-2.40</td>
<td>-1.95</td>
<td>11.58</td>
<td>9.21</td>
<td>-2.36</td>
<td>-2.36</td>
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<tr>
<td>700</td>
<td>156.72</td>
<td>-17.53</td>
<td>-0.77</td>
<td>-2.02</td>
<td>-2.59</td>
<td>-1.95</td>
<td>11.50</td>
<td>8.76</td>
<td>-1.97</td>
<td>-2.52</td>
</tr>
<tr>
<td>1000</td>
<td>91.94</td>
<td>-29.48</td>
<td>-6.15</td>
<td>-2.06</td>
<td>-2.86</td>
<td>-1.95</td>
<td>11.38</td>
<td>8.10</td>
<td>-1.98</td>
<td>-2.77</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>dC₁₁₁/dP</th>
<th>dC₁₁₂/dP</th>
<th>dC₁₂₄/dP</th>
<th>dC₁₁₁/dP</th>
<th>dC₁₁₂/dP</th>
<th>dC₁₂₃/dP</th>
<th>dC₁₄₄/dP</th>
<th>dC₁₆₆/dP</th>
<th>dC₁₆₅/dP</th>
<th>dC₁₆₆/dP</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>-6.81</td>
<td>-0.85</td>
<td>-2.20</td>
<td>-63.94</td>
<td>-1.95</td>
<td>2.24</td>
<td>0.54</td>
<td>-2.02</td>
<td>2.28</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>-6.69</td>
<td>-0.63</td>
<td>-2.19</td>
<td>-51.71</td>
<td>0.54</td>
<td>2.21</td>
<td>0.60</td>
<td>-1.82</td>
<td>2.26</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>-6.58</td>
<td>-0.42</td>
<td>-2.17</td>
<td>-39.91</td>
<td>2.96</td>
<td>2.17</td>
<td>0.65</td>
<td>-1.63</td>
<td>2.24</td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>-6.37</td>
<td>-0.01</td>
<td>-2.15</td>
<td>-17.58</td>
<td>7.55</td>
<td>2.10</td>
<td>0.75</td>
<td>-1.28</td>
<td>2.19</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>-6.09</td>
<td>0.56</td>
<td>-2.11</td>
<td>13.04</td>
<td>13.85</td>
<td>2.01</td>
<td>0.88</td>
<td>-0.79</td>
<td>2.13</td>
<td></td>
</tr>
</tbody>
</table>

Table 4 - The SOPDs of SOECs in $10^{-12}$cm²/dyne and Partial Contraction in $10^{13}$ dyne/cm²

<table>
<thead>
<tr>
<th>Temp(K)</th>
<th>d²C₁₁₁/dP²</th>
<th>d²C₁₁₂/dP²</th>
<th>d²C₁₂₄/dP²</th>
<th>Y₁₁</th>
<th>Y₁₂</th>
<th>Y₄₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>73.05</td>
<td>-2.01</td>
<td>-1.41</td>
<td>24.54</td>
<td>-0.37</td>
<td>3.10</td>
</tr>
<tr>
<td>400</td>
<td>68.24</td>
<td>-1.63</td>
<td>-2.04</td>
<td>20.43</td>
<td>-1.19</td>
<td>2.99</td>
</tr>
<tr>
<td>500</td>
<td>63.87</td>
<td>-1.09</td>
<td>-2.62</td>
<td>16.32</td>
<td>-2.35</td>
<td>2.88</td>
</tr>
<tr>
<td>700</td>
<td>56.07</td>
<td>0.35</td>
<td>-3.67</td>
<td>8.09</td>
<td>-4.67</td>
<td>2.65</td>
</tr>
<tr>
<td>1000</td>
<td>46.19</td>
<td>3.14</td>
<td>-4.91</td>
<td>-4.23</td>
<td>-8.15</td>
<td>2.31</td>
</tr>
</tbody>
</table>

RESULTS AND DISCUSSION

From Table 1, it is clear that the C₁₁ is larger than other second order elastic constants. The values of C₁₁ and C₄₄ increases with temperature, while the value of C₁₂ decreases with temperature. Among the calculated third order elastic constants of LaSe, C₁₂₃ is largest in their absolute values and an order of magnitude larger than the SOECs. Magnitude of other Cᵢᵢᵢ is markedly smaller than those of C₁₂₃. For LaSe, the values of C₁₂₃, C₁₄₄, C₁₆₆ and C₁₆₅ are positive in nature, while C₁₁₁ and C₁₁₂ are negative in nature. There are eleven fourth order elastic constants presented in Table 2. Among the calculated fourth order elastic constants for LaSe, C₁₁₁₁ is the largest in their values. Magnitudes of other Cᵢᵢᵢᵢ are smaller than that of C₁₁₁₁. The values of C₁₁₁₁, C₁₁₂₂, C₄₄₄₄, C₁₄₅₅ and C₁₂₆₆ are positive in nature, while C₁₁₁₂, C₁₁₂₃, C₁₁₄₄, C₁₄₅₆, C₁₄₅₅ and C₁₂₅₅ are negative in nature. Among the calculated first order pressure derivatives of third order elastic constants for LaSe dC₁₁₁/dP is larger than other values in magnitude. The values of dC₁₄₄/dP, dC₁₄₅/dP and dC₁₅₆/dP are positive in nature, while dC₁₁₁/dP, dC₁₁₂/dP and dC₁₆₆/dP are negative in nature. The second order pressure derivatives of C₁₁ at all the temperatures are greater than the derivatives of C₁₂ and C₄₄.

CONCLUSION

There are some temperature variation curves for various elastic constants and their pressure derivatives, which are with a wide temperature range (300-1000 K) and having interval of 50 K. All the curves show a linear relationship between temperature and various
elastic constants. 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 LaSe 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-valent and di-valent crystals; also it can be used to study tri-valent crystals. The same approach can also be used for the study of acoustic properties of mixed crystals [15-19].
REFERENCES