I. Introduction

The LaX, X= S,Se and Te have shown NaCl (B1) FCC to CsCl (B2) under the effect of high pressure. The divalent lanthanum chalcogenides [(LaX, X= S,Se and Te)] are semiconductor and metal in trivalent [1]. The trivalent Lanthanum Chalcogenides have shown the properties of superconductors at 1K [2-4]. The high pressure X-ray diffraction experiment have predicted FCC (B1) to BCC (B2) structure. In the present paper elastic constant such as Young’s modulus, bulk modulus, shear modulus and Poisson ratio in lanthanum chalcogenides [(LaX, X= S,Se and Te)] are calculated with the help of  lattice constants (cij). The Fermi Surface properties of lanthanum chalcogenides [(LaX, X= S,Se and Te)] have been studied by Hass-Van Alphen [5,6]. The elastic constant such as Young’s moduli (Y), bulk moduli (B), shear moduli (G) and Poisson ratio (σ) in lanthanum chalcogenides [(LaX, X= S,Se and Te)] are calculated with help of lattice constants and using the Reuss-Voigt-Hill method [7-9]. The calculated values are close agreement with the experimental results.

II. Theoretical Methodology

The elements sulfur, selenium and telluride are called chalcogens and their compounds are referred as chalcogenides. The crystal structure of lanthanum chalcogenides [(LaX, X= S,Se and Te)] is NaCl (B1) FCC to CsCl (B2) under the effect of high pressure [10-15]. The mechanical properties were studied in terms of lattice constant and Reuss-Voigt-Hill method [7-9]. Various experimental studies have been found lanthanum chalcogenides [(LaX, X= S,Se and Te)] exhibit strongly anharmonic lattice dynamics. The mechanical properties in term of elastic constant such as bulk modulus (B) is given by

\[ B = \frac{1}{2}(c_{11} + 2c_{12}) \]  

Where, \( c_{11} \), and \( c_{12} \) are elastic constants.

The value of Poisson ratio is given by

\[ \sigma = \frac{3B - 2G}{2(3B - G)} \]  

where, \( B \) be the bulk modulus, \( G \) be the average shear modulus and \( G \) be the arithmetic mean of Voigt \( G_v \) and Reuss \( G_r \).

Those values are expressed in term of elastic constants \( (c_{11},c_{12} \, \text{and} \, c_{44}) \) are given by

\[ G_v = \frac{1}{2}(c_{11} - c_{12} + 3c_{44}) \]  

\[ G_r = \frac{5}{3}c_{11} + c_{12}c_{44} \]  

The value of Young’s modulus in term of bulk modulus and shear modulus is given by

\[ Y = \frac{9BG_v}{3B + 4G} \]  

The valence electron, Poisson’s ratio, Work function of La, S, Se and Te are listed in table 1. The calculated values of Young’s moduli (Y), bulk moduli (B), shear moduli (G) and Poisson ratio (σ) in lanthanum chalcogenides [(LaX, X= S,Se and Te)] are listed in table 2, and experimental data have been used from [16-18]. Our calculated values are close agreement with the experimental results.

DOI: 10.9790/4861-1103026263 www.iosrjournals.org 62 | Page
III. Results and Discussion

In this paper, the mechanical properties such as Young’s modulus (Y), bulk modulus (B), shear modulus (G) and Poisson ratio (σ) in lanthanum chalcogenides [(LaX, X = S, Se and Te)] with help of lattice constants and Reuss-Voigt-Hill method have been studied and calculated. Our calculated values of lattice constants are predicted Table 2. The graph plotted lattice parameter Vs poisson ratio of LaS, LaSe and LaTe is shown in fig 1. The graph indicates the semiconducting to metallic behavior. The calculated values of elastic constants are close agreement with experimental result.

Table 1. The valence electron, Poisson’s ratio Work function of La, S, Se and Te

<table>
<thead>
<tr>
<th>Element</th>
<th>Valence electron</th>
<th>Poisson’s ratio</th>
<th>Electron work function (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
<td>5d, 6s</td>
<td>0.288</td>
<td>3.3</td>
</tr>
<tr>
<td>S</td>
<td>3s, 3p</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Se</td>
<td>4s, 4p</td>
<td>0.327</td>
<td>4.72</td>
</tr>
<tr>
<td>Te</td>
<td>5s, 5p</td>
<td>---</td>
<td>4.73</td>
</tr>
</tbody>
</table>

Table 2. The values of lattice parameter, Young’s modulus (Y), shear modulus (G) and Poisson ratio and bulk modulus (B) for in lanthanum chalcogenides [(LaX, X = S, Se and Te)]

<table>
<thead>
<tr>
<th>Compound</th>
<th>Lattice Parameter (a)</th>
<th>c₁₁</th>
<th>c₁₂</th>
<th>c₁₄</th>
<th>Bulk modulus (B) GPa</th>
<th>Young’s Modulus (Y) GPa</th>
<th>Shear Modulus (G) GPa</th>
<th>Poisson ratio (σ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaS</td>
<td>5.85</td>
<td>234</td>
<td>23</td>
<td>25</td>
<td>124</td>
<td>83.6</td>
<td>130.99</td>
<td>0.062</td>
</tr>
<tr>
<td>LaSe</td>
<td>6.05</td>
<td>203</td>
<td>21</td>
<td>22</td>
<td>81.66</td>
<td>74</td>
<td>63.38</td>
<td>0.317</td>
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<tr>
<td>LaTe</td>
<td>6.44</td>
<td>171</td>
<td>12</td>
<td>8</td>
<td>58.33</td>
<td>60.6</td>
<td>88.15</td>
<td>0.495</td>
</tr>
</tbody>
</table>

Fig.1. Lattice Parameter (a) Vs Poisson ratio (σ) for LaS, LaSe and LaTe

References

[17]. S.VonMolnar, T. Penny and F Holtzberg J,Phys.(paris) 37,c4-241 (1976)