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Study of Elastic Constants in Lanthanum Chalcogenides(LaX, X=S, Se and Te)

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Abstract: *In the present paper, Young's moduli (Y),bulk moduli (B),shear moduli (G) and Poisson ratio (σ) of lanthanum chalcogenides [(LaX, X= S,Se and Te)] have been studied and calculatedwith help of lattice constants(c_{ij}) . The calculated values are close agreement with the experimental results.*
Keywords: *Lanthanum chalcogenides, lattice constant and elastic constant*

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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 LanthaniumChalcogenides 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 c_{11},c_{12} and c_{44} lattice constant.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 sulfer, selenium and telluride are called chalcogens and their compounds are referred as chalcogenides.The crystal structure oflanthanum 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 stronglyanharmonic lattice dynamics . The mechanical properties in term of elastic constant such as bulk modulus (B) is given by

$$B=\frac{1}{3}(c_{11}+2\,c_{12}) \qquad (1)$$

Where, c_{11}, and c_{12} are elastic constants.
The value of Poisson ratio is given by

$$\sigma=\frac{3B-2G}{2(3B-G)} \qquad (2)$$

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 ($c_{11}, c_{12}\ and\ c_{44}$) are given by

$$G_v=\frac{1}{5}(c_{11}-c_{12}+3c_{44}) \qquad (3)$$

$$G_R=\frac{5(c_{11}-c_{12})c_{44}}{3(c_{11}-c_{12})+4c_{44}} \qquad (4)$$

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

$$Y=\frac{9\,BG}{3B+G} \qquad (5)$$

The valence electron ,Poissons ratio Work function of La ,S,Se and Te are listed in table1.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.

III. Results and Discussion

In thispaper,the mechanical properties such asYoung'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 arepredicted table 2.The graph plotted lattice parameter Vspoisson ratio of LaS,LaSe and LaTe is shown in fig1. 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, Poissons ratio Work function of La ,S,Se and Te

Element	Valence electron	Poissons ratio	Electron work function (eV)
La	$5d^16s^2$	0.288	3.3
S	$3s^23p^4$	---	---
Se	$4s^24p^4$	0.327	4.72
Te	$5s^25p^4$	---	4.73

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)]

Compound	Lattice Parameter (a)	c_{11}	c_{12}	c_{44}	Bulk modulus (B) GPa Calc.	Bulk modulus (B) GPa Exp [16-18]	Young's Modulus (Y) GPa Calc.	Shear Modulus (G) GPa Calc.	Poisson ratio(σ) Calc.
LaS	5.85	234	23	25	124	83.6	290.63	130.99	0.062
LaSe	6.05	203	21	22	81.66	74	152.250	63.38	0.317
LaTe	6.44	171	12	8	58.33	60.6	263.14	88.15	0.495

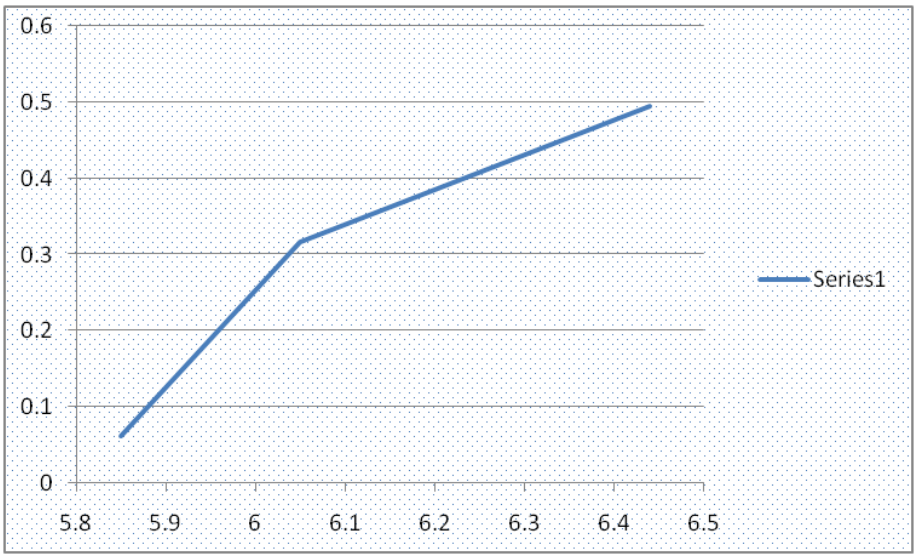

Fig.1.Lattice Parameter (a) VsPoission $ratio$ (σ) for LaS,LaSe and LaTe

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