Analysis of Temperature Dependent Anharmonic Behaviour of Lanthanum Compounds

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Abstract

The study of elastic behavior of a solid is a very important property in fundamental and technical research. In technology, it would tell us about the strength of the materials. In fundamental research, it is of interest because of insight it provides into nature of the binding forces in solids. The relevant elastic constants also relate themselves. The elastic properties of a homogeneous crystal are generally anisotropic. Even in cubic crystals, the relationship between stress and strain depends on orientation of crystal axis relative to stress system. Expression for second, third and higher order elastic constants of solids crystallizing in Lanthanum Compounds are derived from a general potential. As far as known, this study provides the first analysis of higher order elastic constants of Lanthanum Compounds. The third order elastic constants of these materials provide extremely important information, concerning their anharmonic behavior and have therefore been subject of number of theoretical studies. Many useful properties of solid state materials strictly related with their anharmonic behavior.

Keywords: Elastic Constants, Pressure Derivatives, Lanthanum Sulphide, Lanthanum Selenide, Lanthanum Telluride and Partial Contractions.

Introduction

The analysis of experimental data of anharmonic properties is complicated by the fact that the vibrational contributions contain coupling parameter of higher order than the contributions from the cohesive energy. A theory for obtaining anharmonic properties such as higher order elastic constants of materials which possess face centered cubic crystal structure has been developed starting from primary physical parameters viz. nearest neighbour distance and hardness parameter using long- and short- range potentials. The elastic energy density for a deformed crystal can be expanded as a power series of strains using Taylor's series expansion. The coefficients of quadratic, cubic and quartic terms are known as the second, third and fourth order elastic constants respectively. Several physical properties and crystal anharmonicities such as thermal expansion, specific heat at higher temperature, temperature variation of acoustic velocity and attenuation, and the first order pressure derivatives of SOECs, Grüneisen numbers and temperature derivatives of SOECs are directly related to SOECs and TOECs. In last few decade considerable interest has been taken in investigation of anharmonic properties of materials of various kinds [1-10]. In present study higher order elastic constants and the anharmonic properties of LaSe, LaS and LaTe are evaluated at different temperatures from 50 K to up to 1000K.

Formulation

In cubic symmetry, the elastic energy density for a crystal can be expanded up to quartic terms as follows [11].

$$U_0 = U_2 + U_3 + U_4$$
$$= [1/2!]C_{ijk\,l} X_{ij} X_{kl} + [1/3!]C_{ijklmn} X_{ij} X_{kl} X_{mn} + [1/4!]C_{ijklmnpq} X_{ij} X_{kl} X_{mn} X_{pq} \quad (1)$$

Where C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$ are the SOECs, TOECs and FOECs in tensorial form; e_{ij} are the Lagrangian strain components. The SOECs, TOECs and FOECs are as given below:

$$C_{ijkl} = C_{IJ} = (\partial^2 U / \partial e_{ab} \partial e_{cd})_{\varepsilon=0},\ C_{ijklmn} = C_{IJK} = (\partial^3 U / \partial e_{ab} \partial e_{cd} \partial e_{mn})_{\varepsilon=0}$$

and $$C_{ijklmnpq} = C_{IJKL} = (\partial^4 U / \partial e_{ab} \partial e_{cd} \partial e_{mn} \partial e_{pq})_{\varepsilon=0} \quad (2)$$

where C_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations [12].

The free energy density of a crystal at a finite temperature T is

$$U_{Total} = U_0 + U^{vib},\ U^{vib} = [KT / NV_c] \sum_{i=1}^{3sN} \ln 2Sinh(\hbar\omega_i / KT) \quad (3)$$

Where U0 is the internal energy per unit volume of the crystal when all ions are at rest on their lattice points, Uvib is the vibrational free energy, Vc is the volume of the primitive cell, N is the number of the primitive cells in the crystal and s is the number of ions in the elementary cell. Other notations used in this equation have their usual meanings.

An elastic constant consists of two parts as follows:

$$C_{IJ} = C^0_{IJ} + C^{vib}_{IJ},\ C_{IJK} = C^0_{IJK} + C^{vib}_{IJK} \text{ and } C_{IJKL} = C^0_{IJKL} + C^{vib}_{IJKL} \quad (4)$$

The first part is the strain derivative of the internal energy Uo and is known as static elastic constant and the second part is the strain derivative of the vibrational free energy Uvib and is called vibrational elastic constant. The superscript 0 has been introduced to emphasize that the static elastic constants correspond to 0 K.

Evaluation

Using the concept of nearest-neighbour distance and hardness parameter, the elastic constants and pressure derivatives for lanthanum compounds such as LaSe, LaS and LaTe are evaluated at different temperatures (from 50K to 1000K). The temperature variation of C_{ij}, C_{ijk}, C_{ijkl}, dC_{ij}, d^2C_{ij} and Y_{ij} are shown in **Figures 1-6**. In all figures temperature is written as Temperature (K). The values of SOECs, TOECs, FOECs, FOPDs and SOPDs of SOECs and FOPDs of TOECs at room temperature for these crystals are given in **Tables 1 - 5**.

Table 1. Nearest –neighbour distance ($r_{0)}$, hardness parameter (θ) (in 10^{-8} cm) and SOECs in 10^{11} dyne/cm^2 at room temperature for Lanthanum Compounds.

Comp.	r_0	θ	C_{11}	C_{12}	C_{44}
LaSe	2.943	0.345	15.867	5.057	5.190
LaS	2.8116	0.345	16.981	6.204	6.346
LaTe	3.0854	0.345	14.647	4.091	4.215

Table 2. TOECs in 10^{11} dyne/cm^2 at room temperature for Lanthanum Compounds.

Comp.	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
LaSe	-218.129	-1.056	9.010	8.657	8.717	8.344
LaS	-228.937	0.516	10.836	10.389	9.963	10.026
LaTe	-205.874	-1.918	7.429	7.172	7.599	6.907

Table 3. FOECs in 10^{11} dyne/cm^2 at room temperature for Lanthanum Compounds.

Comp.	C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1155}	C_{1255}	C_{1266}	C_{1456}	C_{4444}	C_{4455}
LaSe	2428.90	-16.69	63.46	-19.80	-22.26	96.18	-21.93	113.44	-19.49	116.15	-19.58
LaS	2535.43	8.78	93.60	-23.95	-26.42	117.76	-26.18	138.11	-23.40	141.31	-23.51
LaTe	2301.18	-39.34	36.49	-16.24	-18.55	77.76	-18.26	92.23	-16.13	94.62	-16.20

Table 4. FOPDs of SOECs and TOECs at room temperature for LanthanumCompounds.

Comp.	dC_{11}	dC_{12}	dC_{44}	dC_{111}	dC_{112}	dC_{123}	dC_{144}	dC_{166}	dC_{456}
LaSe	-6.826	-0.849	-2.204	-64.017	-1.916	2.246	0.544	-2.020	2.288
LaS	-6.195	-1.037	-2.247	-60.500	-3.721	2.339	0.620	-2.238	2.367
LaTe	-7.461	-0.695	-2.165	-67.302	0.089	2.159	0.470	-1.805	2.213

Table 5. The SOPDs of SOECs in 10^{-10} (dyne/cm^2)$^{-1}$ and Partial Contraction (Y) in 10^{13}(dyne/cm^2) for at room temperature Lanthanum Compounds.

Comp.	d^2C_{11}	d^2C_{12}	d^2C_{44}	Y_{11}	Y_{12}	Y_{44}
LaSe	0.735	-0.020	-0.014	24.494	-0.055	3.093
LaS	0.550	-0.015	-0.000	27.099	0.850	3.804
LaTe	0.969	0.032	-0.031	21.843	-0.869	2.484

Results and Discussions:

The SOECs in 10^{11} dyne/cm^2 at room temperature for lanthanum compounds such as LaSe, LaS, and LaTe are shown in **Table 1**. It is clear from this table that all the SOECs are positive in nature. The values of C_{ij}'s are varying from 4.091×10^{11}dyne/cm^2 to 16.981×10^{11}dyne/cm^2. From **Figure 1** the values of second order elastic constant C_{11} increased with increas in temperature for all these lanthanum compounds LaSe, LaS and LaTe, and the value of C_{44} is also increased with increasing of temperature while the values of C_{12} decrease with increasing of temperature for these lanthanum compounds.

The higher order elastic constants are strongly related to other anharmonic properties; such as thermal expansion, thermo elastic constants and thermal conductivity. The knowledge of TOECs may provide further critical data for testing the machines for non-destructive-testing. Third order elastic constants play an important role in solid-state physics. These elastic constants are used to compute ultrasonic parameters [13, 14] such as ultrasonic velocities, thermal relaxation time etc. The variation of elastic constants [15-17] with respect to pressure can reveal many important features of the short range forces at high pressure. The ultrasonic studies [18-20] can provide interesting information on the specificities of ion-solvent interaction related to the structure of the solute and the reciprocal effects which arise in the solvent.

The present results of TOECs in10^{11} dyne/cm^2 at room temperature for LaSe, LaS, and LaTe are shown in **Table 2**. From **Figure 2** shows that C_{111} is increased with increase in temperature.

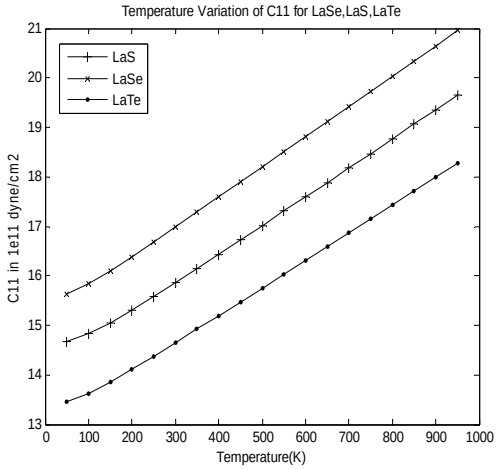

Figure 1 Temperature Variation of C_{11} for LaSe, LaS and LaTe

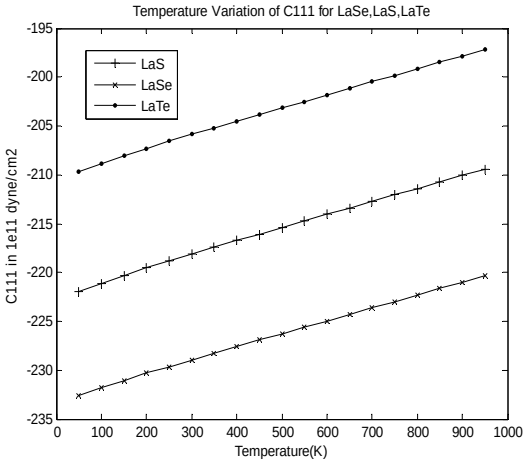

Figure 2 Temperature Variation of C_{111} for LaSe, LaS and LaTe

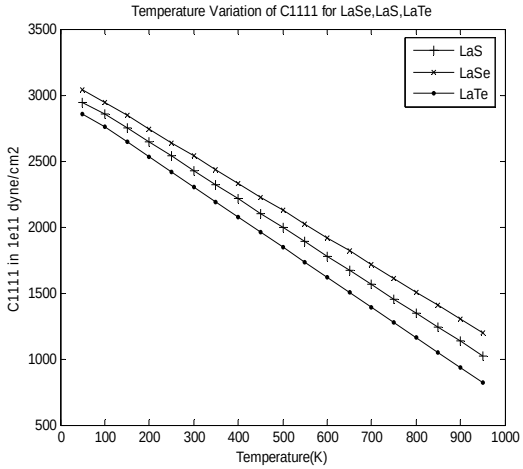

Figure 3 Temperature VariationofC$_{1111}$ for LaSe, LaS and LaTe

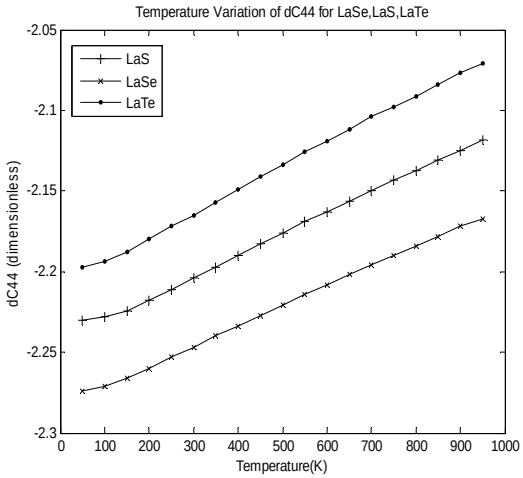

Figure 4 Temperature Variation of dC_{44}/dpforLaSe, LaS and LaTe

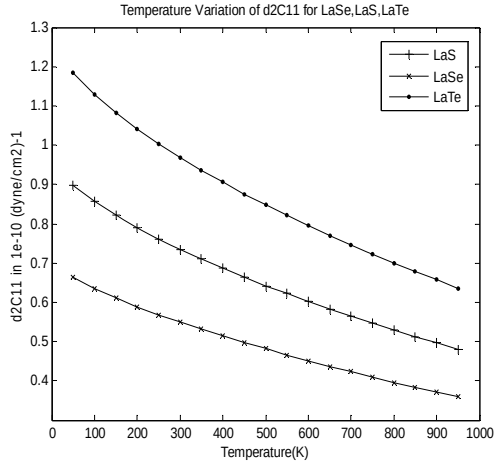

Figure 5 Temperature Variation of d^2C_{11}/dp^2 for LaSe, LaS and LaTe

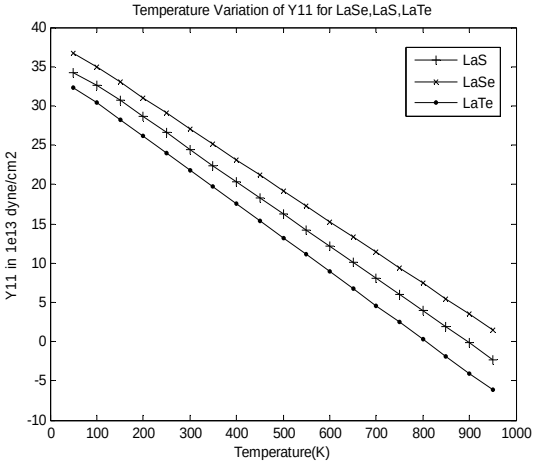

Figure 6 Temperature Variation of Y_{11} for LaSe, LaS and LaTe

We also deduce that the value of C_{112} is decrease for all lanthanum compounds such as LaSe, LaS, and LaTe with increase in temperature, and C_{123}, C_{144} and C_{166} increases for all these lanthanum compounds as temperature increases. We have already discussed the temperature variation of second and third order elastic constants of lanthanum compounds such as LaSe, LaS and LaTe. The FOECs for LaSe, LaS, and LaTe are given in **Table 3**. The Partial Contractions in 10^{13} dyne/cm^2 for LaSe, LaS and LaTe are given in **Table 5**. Calculated results of fourth order elastic constant C_{1111} at different temperatures are reported in **Figure 3**. Other results are also given in **Table 3**.

The FOPDs and SOPDs of the SOECs of lanthanum compounds such as LaSe, LaS and LaTe are presented in **Table 4** and **Table 5**. Calculated results of first order pressure derivative of C_{44} at different temperatures are reported in **Figure no. 4.** It is clear that C_{44} is increased with increasing of temperature, and we also find that the FOPDs of C_{12} and C_{44} also increased with increasing of temperature for all these lanthanum compounds and The values of dC_{111}/dp, dC_{112}/dp, dC_{144}/dp, dC_{166}/dp increase with increasing of temperature, while the values of dC_{123}, dC_{456} decrease with increasing of temperature for all these lanthanum compounds, whose values are given in **Table 4.** Calculated results of second order pressure derivative of C_{11} at different temperatures are reported in **Figure 5** and results of Y_{11} are also reported in **Figure 6**. The new data may provide a further chance to improve the theoretical models developed recently for the interpretation of the behavior of elastic constants in higher temperature region.

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