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PRESSURE DERIVATIVS OF HIGHER ORDER ELASTIC CONSTANTS OF CALCIUM OXIDE SINGLE CRYSTAL IN HIGH TEMPERATURE RANGE

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ABSTRACT

Rocks are complicated heterogeneous materials with microstructures that scatter acoustic or seismic waves. The anharmonic properties play an important role in the study that how the rock formed. In this work, an attempt has been made to evaluate higher order elastic constants for CaO at an elevated temperature from 50 K to 2600 K. The data of second order elastic constants (SOECs), third order elastic constants (TOECs) and fourth order elastic constants (FOECs) are used to evaluate the first order pressure derivatives (FOPDs) of SOECs and TOECs, second order pressure derivatives (SOPDs) of SOECs and partial contractions. While evaluating these properties it is assumed that the crystal structure does not change during temperature variation. When the values of second and third order elastic constants and density for any material at a particular temperature are known; one may get Grüneisen numbers, ultrasonic velocities for longitudinal and shear waves in different crystallographic directions which give important information about its anharmonic properties. The data of these oxides obtained through different techniques also give important and valuable information about internal structure and inherent properties of materials and can be used in future for different industrial purposes and further investigations of isostructural oxides.

Keywords: SOPDs, CaO, elastic constants, etc.

INTRODUCTION

The information about anharmonic properties is valuable in understanding nature of short range forces in crystals. The efforts for evaluating anharmonic properties have been made for mono-valent rock-salt structured materials discussed by some investigators. Elastic properties of divalent compounds are also equally important because they relate to the various fundamental solid state phenomena such as inter – atomic potentials, equation of state and phonon spectra. If the values of second order elastic constants and density at a particular temperature are known for any substance, one may obtain ultrasonic velocities for longitudinal and shear waves which give an important information about its anharmonic properties.Elastic properties are linked thermodynamically with specific heat, thermal expansion, and Debye temperature and Grüneisen parameters.

The elastic constants play primary role for understanding the anharmonic and non linear properties of solids[1-3]. In the last few years studies of anharmonic properties of solids have attracted the attention of the physicists since they provide much valuable information regarding crystal dynamics[4-7]. A number of theoretical and experimental 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 of (FOPDs) of SOECs and TOECs, second order pressure derivatives of second order elastic constants (SOPDs) of SOECs etc. of several ionic crystals[8]. No complete experimental or theoretical efforts have been made so for in obtaining the temperature variation of anharmonic properties of divalent crystals having various crystal structures. The elastic energy density for a deformed crystal can be expanded as a power series of strains using Taylor's series expansion[9]. The coefficients of quadratic, cubic and quartic terms are known as SOECs, TOECs and FOECs 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 FOPDs of SOECs and Gruneisen numbers are directly related to SOECs and TOECs. While discussing higher order anharmonicities such as the FOPDs of TOECs, the SOPDs of SOECs, partial contractions and deformation of crystals under large forces, the FOECs are to be considered extensively. The present paper is mainly focussed on the study of temperature

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variation of higher order elastic constants and their pressure derivatives up to an elevated temperature up to near melting point for Calcium oxide (CaO) crystals using Born-Mayer and Coulomb potential starting from the nearest neighbor distance and hardness parameter.

Theoretical Approach

The elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as shown below[10];

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

Where C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$ are the SOECs, TOECs and FOECs in tensorial form; α_{ij} are the Lagrangian strain components. TheSOECs, TOECs and FOECs are as givenbelow:

$$C_{ijkl} = C_{IJ} = \left(\frac{\partial^2 U}{\partial\alpha_{ij}\partial\alpha_{kl}}\right)_{\alpha=0}$$

$$C_{ijklmn} = C_{IJK} = \left(\frac{\partial^3 U}{\partial\alpha_{ij}\partial\alpha_{kl}\partial\alpha_{mn}}\right)_{\alpha=0}$$

$$C_{ijklmnpq} = C_{IJKL} = \left(\frac{\partial^4 U}{\partial\alpha_{ij}\partial\alpha_{kl}\partial\alpha_{mn}\partial\alpha_{pq}}\right)_{\alpha=0} \quad \text{and...(2)}$$

whereC_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations[11]. The free energy densityof a crystal at a finite temperature T is

$$U_{Total} = U_0 + U^{vib},$$

$$\text{Where} \quad U^{vib} = \frac{KT}{NV_c}\sum_{i=1}^{3sN}\ln 2Sinh\left(\frac{\hbar\omega_i}{KT}\right) \quad \text{...(3)}$$

Where U_0 is the internal energy per unit volume of the crystal when all ions are at rest on their lattice points, U^{vib} is the vibrational free energy, V_c 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:

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{vib}, \qquad C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib} \qquad \text{and}$$

$$C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{vib} \qquad \text{...(4)}$$

The first part is the strain derivative of the internal energy U_o and is known as static elastic constant and the second part is the strain derivative of the vibrational free energy U^{vib} and is called vibrational elastic constant. The superscript 0 has been introduced to emphasize that the static elastic constants correspond to absolute zero temperature.

RESULTS AND DISCUSSIONS

The SOECs, TOECs and FOECs in 10^{10} N/m^2 at room temperature for CaO are given in Tables 1 - 2. The FOPDs of the SOECs and TOECs are presented in Table 3. The SOPDs of the SOECs in 10^{-9} m^2/N and Partial Contractions in 10^{12} N/m^2 are also shown in Table 4. The temperature variation of anharmonic properties SOECs, TOECs and FOECs, FOPDs of SOECs, the SOPDs of SOECs and partial contractions for CaO are represented graphically in Figs. 1 - 6. 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 SOECs and TOECs along with other physical properties may provide further critical data for testing the machines for non-destructive-testing. These elastic constants are used to compute ultrasonic parameters such as ultrasonic velocities, thermal relaxation time etc[12-14]. 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] can provide interesting information on the specificities of ion-solvent interaction related to the structure of the solute and the reciprocal effects which arises in the solvent and the role of collinear and noncolinear phonons in anharmonic scattering processes and in ultrasonic attenuation for different structured solids[19].

Table 1. SOECs in 10^{10} N/m^2 for CaO crystal at room temperature

Melting Point (K)	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
2843K	20.674	12.527	12.718	-252.887	-65.105	20.349	19.439	-51.266	4.713

Table 2. The FOECs in 10^{10} N/m^2 for CaO crystal at room temperature

C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1155}	C_{1255}	C_{1266}	C_{1456}	C_{4444}	C_{4455}
2694.38	133.03	240.10	-12.23	-44.45	230.24	-48.21	267.05	-44.04	271.24	-44.28

Table 3. The FOPDs of SOECs and TOECs for CaO crystal at room temperature

dC_{11}/dP	dC_{12}/dP	dC_{44}/dP	dC_{111}/dP	dC_{112}/dP	dC_{123}/dP	dC_{144}/dP	dC_{166}/dP	dC_{456}/dP
-7.383	-3.280	0.628	-47.9307	-4.052	2.773	0.994	1.462	2.748

Table 4. The SOPDs of SOECs in 10^{-9} m^2/Nand partial contractions in 10^{12} N/m^2 for CaO crystal at room temperature

d^2C_{11}/dP^2	d^2C_{12}/dP^2	d^2C_{44}/dP^2	Y_{11}	Y_{12}	Y_{44}
0.692	0.163	0.136	36.149	5.168	7.537

CONCLUSION

It may state that all the SOECs are positive in nature. For CaO crystals the value of C_{11} increases and the value of C_{12} and C_{44} decrease as temperature increases and are represented in Fig. 1. For Calcium remaining constant. The variation of first three C_{111}, C_{112} and C_{123} are given in Fig. 2. The value of C_{1111}, C_{1112}, C_{1122}, C_{1144},C_{1155}, C_{1255}, C_{1266}, C_{4444} and C_{4455} decreases as temperature increases, and the value of C_{1123} increases as temperature increases. The value of C_{1456} remains constant. The graphical representations for first three are given in Fig. 3. The value of dC_{11}/dp and dC_{12}/dpdecreases and the value of dC_{44}/dp increases as temperature increases. The value of dC_{111}/dp, dC_{112}/dp, dC_{144}/dp, dC_{166}/dp and dC_{456}/dpincreases as temperature increases, and the value of dC_{123}/dpdecrease as temperature increases.

oxide, the values of C_{111}, C_{112} and C_{166} are negative in nature, while C_{123}, C_{144} and C_{456} are positive in nature. The values of C_{111}, C_{123}, C_{144} and C_{166} increases, the value of C_{112},decreases as temperature increases, C_{456}

The variation of FOPDs of SOECs is given in Fig. 4. The value of d^2C_{11}/dp^2 and d^2C_{44}/dp^2 decreases and d^2C_{12}/dp^2 increases as temperature increases and are presented in Fig. 5. The value of all partial contractions Y_{11}, Y_{12} and Y_{44} decreases as temperature increases but Y_{11} decreases very sharply, which is presented in Fig. 6. The data obtained in present investigation will be helpful to those workers who are engaged in studying the temperature variation of anharmonic properties[20–24] of solids at higher temperatures.

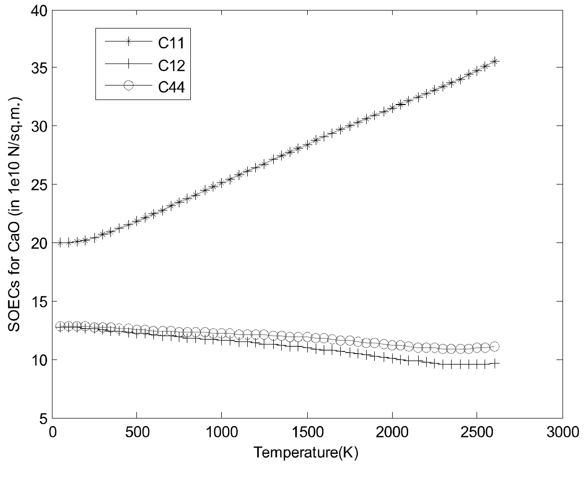

Fig.1 SOECs vs. Temperature

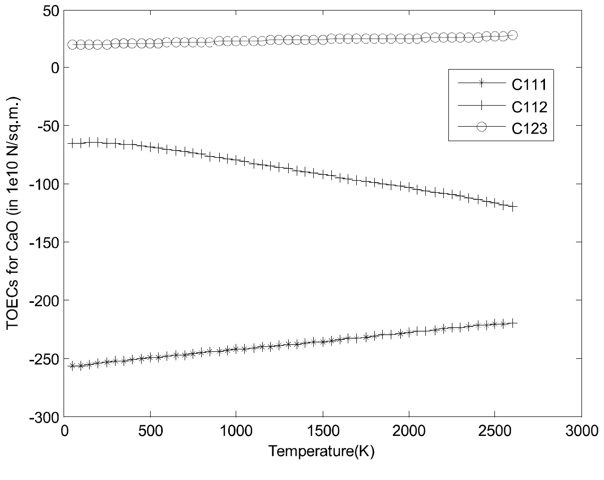

Fig.2 TOECs vs. Temperature

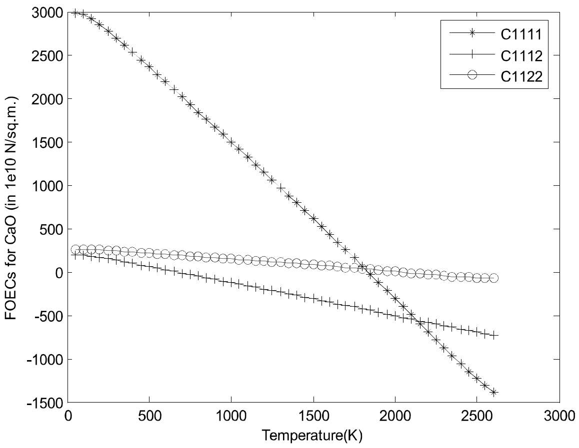

Fig.3 FOECs vs. Temperature

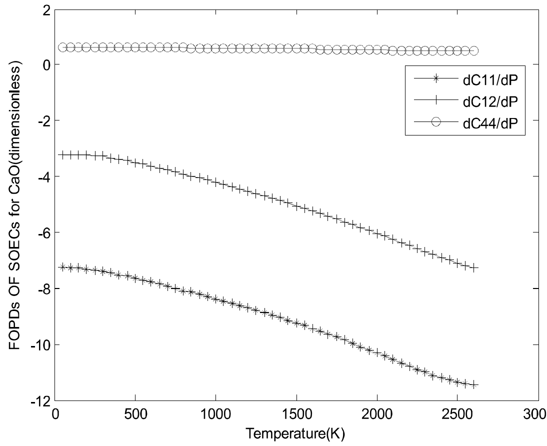

Fig.4 FOPD of SOECs vs. Temperature

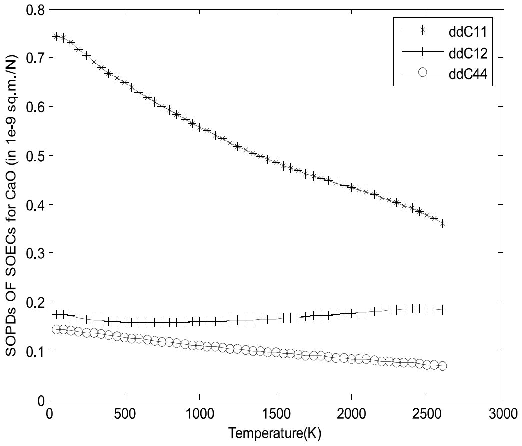

Fig.5 SOPD of SOECs vs. Temperature

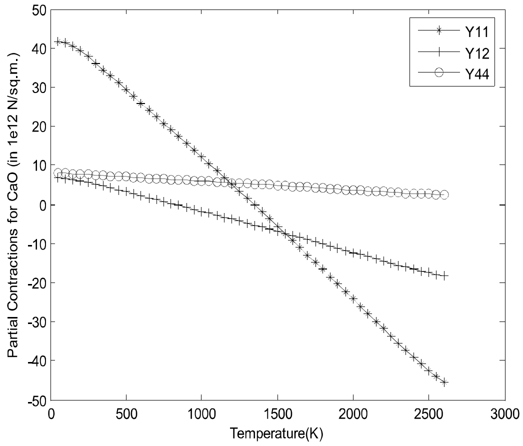

Fig.6 Partial Contractions vs. Temperature

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