



## Temperature Dependence of Pressure Derivatives of Higher Order Elastic Constants of TeO Crystal<sup>†</sup>

JITENDRA KUMAR<sup>1,\*</sup>, KAILASH<sup>2</sup>, VIRENDRA KUMAR<sup>2</sup> and A.K. CHAUDHARY<sup>3</sup>

<sup>1</sup>Department of Physics, Government Girls Post Graduate College, Banda-210 001, India

<sup>2</sup>Department of Physics, BN Post Graduate College, Rath, Hamirpur-210 431, India

<sup>3</sup>Department of Physics, Atarra Post Graduate College, Atarra-210 201, India

\*Corresponding author: Fax: +91 5192 224499; Tel: +91 9839168210; E-mail: jitendra\_sharma50@yahoo.com

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A proper and systematic evaluation of the elastic constants of isostructural oxides and their dependence on temperature provides the fundamental data for determining the characteristics of cation-oxygen bonding interactions, which are pertinent to the understanding and theoretical modelling of more complicated oxide compounds. The information about higher order elastic constants is valuable in understanding nature of short range forces in crystals. Tellurium oxide is a divalent crystals and possess FCC crystal structure. In this work, an attempt has been made to evaluate higher order elastic constants for tellurium oxide at an elevated temperature starting from 50 K to near its melting point. The melting point for tellurium oxide is 643 K. The data of second, third and fourth order elastic constants (SOECs, TOECs and 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. 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 divalent FCC structured solids and other isostructural oxides.

**Key Words:** Anharmonic properties, Higher order elastic constants, Pressure derivatives, Divalent crystals, Partial contractions.

### INTRODUCTION

Rocks are complicated heterogeneous materials with microstructures that scatter acoustic or seismic waves. At the laboratory (ultrasonic) scale, these microstructures are primarily cracks and grain boundaries. The scattering of waves from these boundaries is generally considered noise in geophysical applications, but these scattered wave fields may give insight into how the rock formed, the environment in which it formed, its state of stress, fluid saturation *etc.* The anharmonic properties play an important role in this type of studies. The efforts for evaluating anharmonic properties have been made for monovalent 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 the solids<sup>1-3</sup>. In the last few years, anharmonic properties of solids have attracted the attention of the physicists since they provide much valuable information regarding crystal dynamics<sup>4-6</sup>. 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<sup>7</sup>. No complete experimental or theoretical efforts have been made so far 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<sup>8</sup>. The

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

## EXPERIMENTAL

The elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as shown below<sup>9</sup>:

$$U_0 = U_2 + U_3 + U_4$$

$$= [1/2!] C_{ijkl} \alpha_{ij} \alpha_{kl} + [1/3!] C_{ijklmn} \alpha_{ij} \alpha_{kl} \alpha_{mn} + [1/4!] C_{ijklmnpq} \alpha_{ij} \alpha_{kl} \alpha_{mn} \alpha_{pq} \quad (1)$$

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

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

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

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

where  $C_{IJ}$ ,  $C_{IJK}$  and  $C_{IJKL}$  are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations<sup>10</sup>. The free energy density of a crystal at a finite temperature  $T$  is:

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

where,

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

where  $U_0$  is the internal energy per unit volume of the crystal when all ions are at rest on their lattice points,  $U^{\text{vib}}$  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:

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

The first part is the strain derivative of the internal energy  $U_0$  and is known as static elastic constant and the second part is the strain derivative of the vibrational free energy  $U^{\text{vib}}$  and is called vibrational elastic constant. The superscript 0 has been introduced to emphasize that the static elastic constants correspond to absolute zero temperature.

**Evaluation:** The theory for the calculation of different anharmonic properties of the substances possessing FCC crystal structures is given in the preceding section. The SOECs, TOECs and FOECs for TeO crystal are evaluated from 50 K to an elevated temperature (near melting point). Selecting a few data obtained in this study, the values of SOECs, TOECs and FOECs at room temperature are given in Tables 1-3. The FOPDs of SOECs and TOECs, the SOPDs of SOECs and partial contractions are evaluated utilizing data of Tables 1-3 and the results are shown in Tables 4 and 5. All these results are presented graphically in Figs. 1-6.

TABLE-1  
NEAREST NEIGHBOUR DISTANCE ( $r_0$ ) AND HARDNESS  
PARAMETER ( $q$ ) IN  $10^{-10}$  m AND SOECs IN  $10^{10}$  N/m<sup>2</sup>  
AT ROOM TEMPERATURE

| Property | m.p. (k) | $r_0$  | $q$   | $C_{11}$ | $C_{12}$ | $C_{44}$ |
|----------|----------|--------|-------|----------|----------|----------|
| Value    | 643      | 2.7865 | 0.345 | 20.711   | 22.109   | 22.346   |

TABLE-2  
TOECs IN  $10^{10}$  N/m<sup>2</sup> AT ROOM TEMPERATURE

| Property | $C_{111}$ | $C_{112}$ | $C_{123}$ | $C_{144}$ | $C_{166}$ | $C_{456}$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Value    | -234.110  | -102.256  | 33.826    | 32.482    | -88.531   | 31.679    |

## RESULTS AND DISCUSSION

The SOECs, TOECs and FOECs in  $10^{10}$  N/m<sup>2</sup> at room temperature for TeO are given in Tables 1-3. The FOPDs of the SOECs and TOECs are presented in Table-4. The SOPDs

TABLE-3  
FOECs IN  $10^{10}$  N/m<sup>2</sup> AT ROOM TEMPERATURE

| Property | $C_{1111}$ | $C_{1112}$ | $C_{1122}$ | $C_{1123}$ | $C_{1144}$ | $C_{1155}$ | $C_{1255}$ | $C_{1266}$ | $C_{1456}$ | $C_{4444}$ | $C_{4455}$ |
|----------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| Value    | 2392.0     | 301.0      | 434.1      | -77.23     | -74.48     | 387.4      | -79.45     | 447.1      | -74.01     | 452.6      | -74.41     |

TABLE-4  
FOPDs OF SOECs AND TOECs AT ROOM TEMPERATURE

| Property | $dC_{11}/dP$ | $dC_{12}/dP$ | $dC_{44}/dP$ | $dC_{111}/dP$ | $dC_{112}/dP$ | $dC_{123}/dP$ | $dC_{144}/dP$ | $dC_{166}/dP$ | $dC_{456}/dP$ |
|----------|--------------|--------------|--------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Value    | -5.725       | -3.414       | 0.967        | -33.881       | -6.652        | 3.096         | 1.256         | 1.596         | 3.044         |

TABLE-5  
SOPDs of SOECs IN  $10^9$  (N/m<sup>2</sup>)<sup>-1</sup> AND PARTIAL CONTRACTIONS IN  $10^{12}$  N/m<sup>2</sup> AT ROOM TEMPERATURE

| Property | $d^2C_{11}/dP^2$ | $d^2C_{12}/dP^2$ | $d^2C_{44}/dP^2$ | $W_{11}$ | $W_{12}$ | $W_{44}$ |
|----------|------------------|------------------|------------------|----------|----------|----------|
| Value    | 0.380            | 0.124            | 0.110            | 43.101   | 10.842   | 12.728   |

of the SOECs in  $10^{-9} \text{ m}^2/\text{N}$  and partial contractions in  $10^{12} \text{ N}/\text{m}^2$  are also shown in Table-5. The temperature variation of anharmonic properties SOECs, TOECs and FOECs, FOPDs of SOECs, the SOPDs of SOECs and partial contractions for TeO 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.*<sup>11-13</sup>. The variation of elastic constants<sup>14-16</sup> with respect to pressure can reveal many important features of the short range forces at high pressure. The ultrasonic studies<sup>17</sup> 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 noncollinear phonons in anharmonic scattering processes and in ultrasonic attenuation for different structured solids<sup>18</sup>.

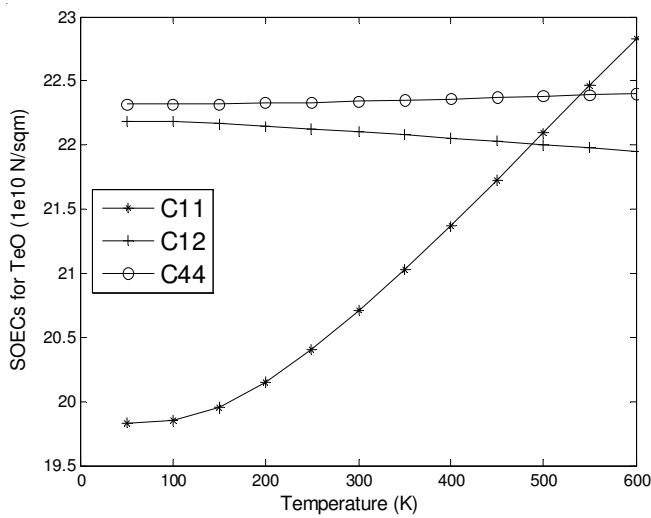


Fig. 1. Temperature variation of SOECs

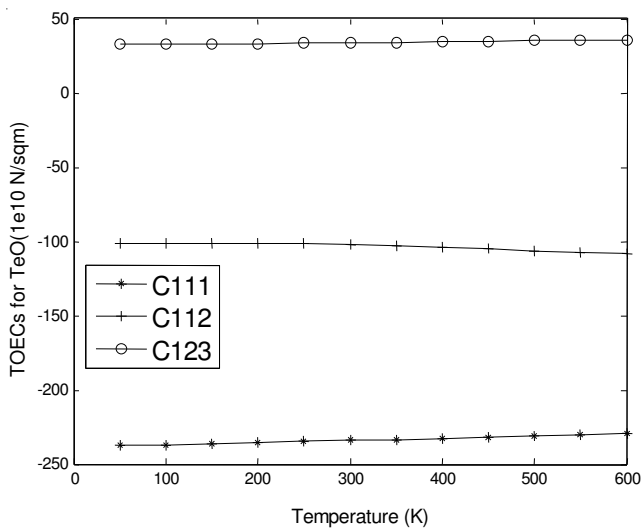


Fig. 2. Temperature variation of TOECs

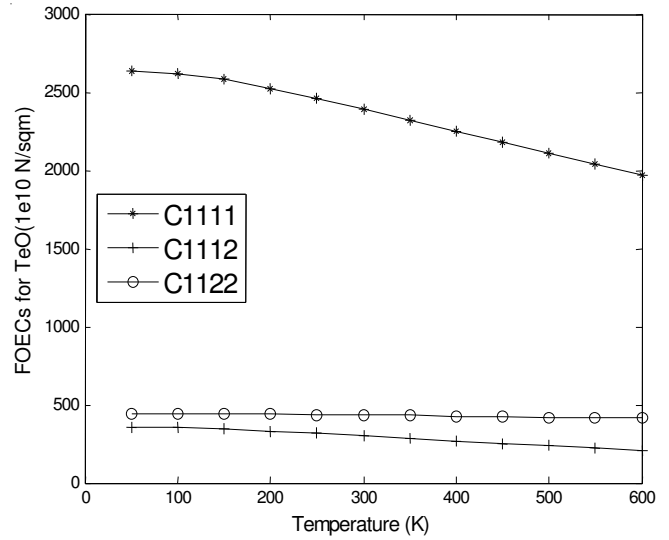


Fig. 3. Temperature variation of FOECs

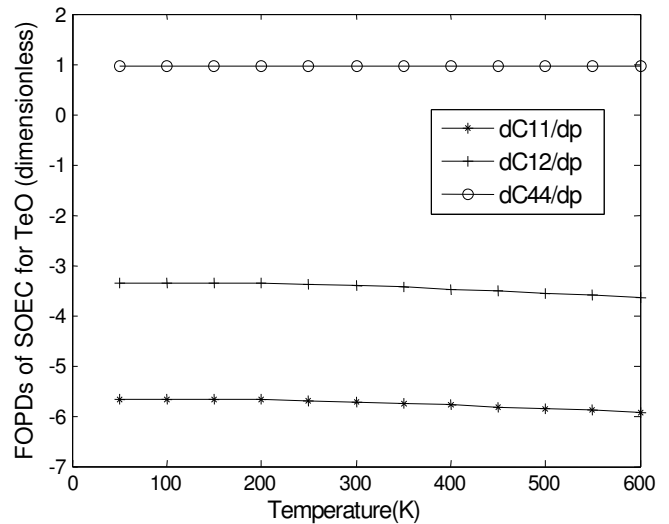


Fig. 4. Temperature variation of FOPDs of SOECs

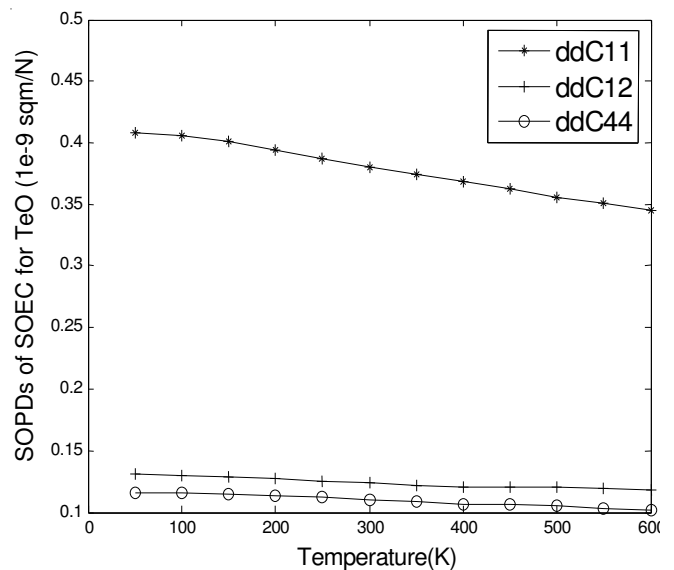


Fig. 5. Temperature variation of SOPDs of SOECs

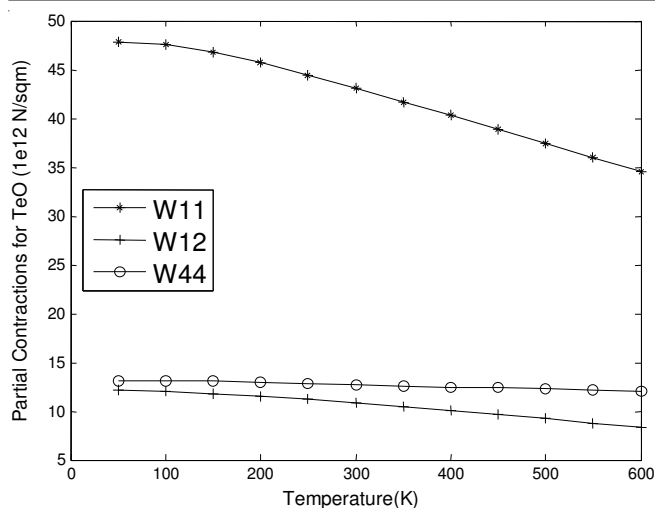


Fig. 6. Temperature variation of partial contractions

It may state that all the SOECs are positive in nature. For TeO crystals the value of  $C_{11}$  and  $C_{44}$  increases and the value of  $C_{12}$  decrease as temperature increases and are represented in Fig. 1. for tellurium oxides, 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,  $C_{456}$  remaining constant. The variation of  $C_{111}$ ,  $C_{112}$  and  $C_{123}$  are given in Fig. 2. For fourth order elastic constants, 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  $dC_{12}/dp$  decreases and the value of  $dC_{44}/dp$  increases as temperature increases. The value of  $dC_{111}/dp$ ,  $dC_{144}/dp$ ,  $dC_{166}/dp$  and  $dC_{456}/dp$  increases as temperature increases and the value of  $dC_{123}/dp$  decrease as temperature increases. The variation of FOPDs of SOECs are 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  $W_{11}$ ,  $W_{12}$  and  $W_{44}$  decreases as temperature increases but  $W_{11}$  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<sup>19,20</sup> of solids at higher temperatures.

## Conclusion

On the basis of above discussion, the following conclusions can be drawn: The new data may provide a further chance to improve the theoretical models developed recently for the interpretation of the behaviour of elastic constants in higher temperature region.

The method taken up for theoretical evaluation of SOEC and TOEC is also justified for this divalent oxide crystal.

Through theory explains the temperature dependence of the elastic constants, a microscopic understanding is lacking, such efforts are under way.

But as the non availability of experimental data, a detailed discussion of these properties may be left for a later investigation when the main effects are better understood.

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