Temperature Variation of Anharmonic Properties of Tellurium Oxide Single Crystal

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ABSTRACT

The study of higher order elastic constants has gained new horizons with the development of material science as they play primary role for understanding the anharmonic and non linear properties of solids. The information about these constants is valuable in understanding nature of short range forces in crystals. The elastic energy density for a deformed crystal can be expanded as a power series of strains using Taylor's series expansion. One can get this expansion starting from nearest neighbour distance and hardness parameter utilizing Coulomb and Born-Mayer type central force interactions for face centred cubic crystals. The coefficients of the quadratic, cubic and quartic terms are known as the second, third and fourth order elastic constants (SOECs, TOECs and FOECs) respectively. When the values of second and third order elastic constants and density for any material at a particular temperature are known; one may get ultrasonic velocities for longitudinal and shear waves in different crystallographic directions which give important information about its anharmonic properties. While obtaining higher order anharmonicities such as Grüneisen numbers, the first order pressure derivatives of second order elastic constants (FOPDs of SOECs), the first order pressure derivatives of third order elastic constants (FOPDs of TOECs), the second order pressure derivatives of second order elastic constants (SOPDs of SOECs), partial contractions and deformation of crystals under large forces, the third and fourth order elastic constants are considered extensively. 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 Tellurium Oxide (TeO) is a divalent crystals and possess FCC crystal structure. In this work, an attempt has been made to evaluate higher order elastic constants for TeO at an elevated temperature starting from 50K to near its melting point. The melting point for TeO is 643 K. The data of SOECs, TOECs and FOECs are used to evaluate the FOPDs of SOECs and TOECs, 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.

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 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 variation of higher order elastic constants and

their pressure derivatives up to an elevated temperature up to near melting point for Tellurium oxide (TeO) crystals using Born-Mayer and Coulomb potential starting from the nearest neighbour distance and hardness parameter.

FORMULATION

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

$U_0 = U_2 + U_3 + U_4$

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

$= [1/2] \ C_{11} \ (\alpha_{11}^2 + \alpha_{22}^2 + \alpha_{33}^2) + C_{12} \ (\alpha_{11}\alpha_{22} + \alpha_{22} \ \alpha_{33} + \alpha_{33} \ \alpha_{11})$

$\quad + 2C_{44} \ (\alpha_{12}^2 + \alpha_{23}^2 + \alpha_{31}^2) + [1/6 \ ] \ C_{111} \ (\alpha_{11}^3 + \alpha_{22}^3 + \alpha_{33}^3)$

$\quad + [1/2] \ C_{112}[\alpha_{11}^2(\alpha_{22} + \alpha_{33}) + \alpha_{22}^2 \ (\alpha_{33} + \alpha_{11}) + \alpha_{33}^2 \ (\alpha_{11} + \alpha_{22})]$

$\quad + C_{123} \ \alpha_{11} \ \alpha_{22} \ \alpha_{33} + 2C_{144} \ (\alpha_{11} \ \alpha_{23}^2 + \alpha_{22} \ \alpha_{31}^2 + \alpha_{33} \ \alpha_{12}^2)$

$\quad + 2C_{166} \ [\alpha_{12}^2 \ (\alpha_{11+} \ \alpha_{22}) + \alpha_{23}^2 \ (\alpha_{22}+\alpha_{33}) + \alpha_{31}^2 \ (\alpha_{33} + \alpha_{11})]$

$\quad + 8C_{456} \ \alpha_{12} \ \alpha_{23} \ \alpha_{31} + [1/24] \ C_{1111} \ (\alpha_{11}^4 + \alpha_{22}^4 + \alpha_{33}^4)$

$\quad + [1/6] \ C_{1112} \ [\alpha_{11}^3 \ (\alpha_{22} + \alpha_{33}) + \alpha_{22}^3 \ (\alpha_{33} + \alpha_{11}) + \alpha_{33}^3 \ (\alpha_{11}+ \alpha_{22})]$

$\quad + [1/4] \ C_{1122} \ (\alpha_{11}^2 \ \alpha_{22}^2 + \alpha_{22}^2 \ \alpha_{33}^2 + \alpha_{33}^2 \ \alpha_{11}^2) + [1/2] \ C_{1123} \ \alpha_{11} \ \alpha_{22} \ \alpha_{33} \ (\alpha_{11} + \alpha_{22} + \alpha_{33})$

$\quad + C_{1144} \ (\alpha_{11}^2 \ \alpha_{23}^2 + \alpha_{22}^2 \ \alpha_{31}^2 + \alpha_{33}^2 \ \alpha_{12}^2)$

$\quad + C_{1155} \ (\alpha_{11}^2 \ (\alpha_{31}^2 + \alpha_{12}^2) + \alpha_{22}^2 \ (\alpha_{12}^2 + \alpha_{23}^2) + \alpha_{33}^2 \ (\alpha_{23}^2 + \alpha_{31}^2)]$

$\quad + 2C_{1255} \ (\alpha_{11} \ \alpha_{22} \ (\alpha_{23}^2 + \alpha_{31}^2) + \alpha_{22} \ \alpha_{33} \ (\alpha_{31}^2 + \alpha_{12}^2) + \alpha_{33} \ \alpha_{11} \ (\alpha_{12}^2 + \alpha_{23}^2)]$

$\quad + 2C_{1266} \ (\alpha_{11} \ \alpha_{22} \ \alpha_{12}^2 + \alpha_{22} \ \alpha_{33} \ \alpha_{23}^2 + \alpha_{33} \ \alpha_{11} \ \alpha_{31}^2)$

$\quad + 8C_{1456} \ \alpha_{12} \ \alpha_{23} \ \alpha_{31} \ (\alpha_{11} + \alpha_{22} + \alpha_{33}) + [2/3] \ C_{4444} \ (\alpha_{12}^4 + \alpha_{23}^4 + \alpha_{31}^4)$

$\quad + 4C_{4455} \ (\alpha_{12}^2 \ \alpha_{23}^2 + \alpha_{23}^2 \ \alpha_{31}^2 + \alpha_{31}^2 \ \alpha_{12}^2)$ (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. 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 $\quad C_{ijklmnpq} = C_{IJKL} = \left(\frac{\partial^4 U}{\partial \alpha_{ij} \partial \alpha_{kl} \partial \alpha_{mn} \partial \alpha_{pq}} \right)_{\alpha=0}$ (2)

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

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

Where

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

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{vib} ,$$

$$C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib}$$

and $$C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{vib} \tag{4}$$

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.

The energy density of the non- deformed crystal is expressed as:

$$U_0 = \frac{1}{2V_c} \sum_{v=1}^{s} \sum_{\substack{m \neq o \\ |u \neq v|}} Q_{uv}(R_{uv}^{mo}) = \sum{}' \frac{Q_{uv}(R)}{2V_c} \tag{5}$$

Where R_{uv}^{mo} is the distance between the v-th ion in the o-th cell and the u-th ion in the m-th cell and Q_{uv} is the interaction potential between the ions. The indices (v, o) and (u, m) are sometimes dropped when no confusion occurs. One assumes that Q_{uv} is the sum of the long-range Coulomb and the short-range Börn-Mayer potentials.

$$Q_{uv}(r_0) = \pm \left(\frac{e^2}{r_0} \right) + A \exp\left(\frac{-r_0}{\eta} \right) \tag{6}$$

Where e is the electric charge, $\pm$ sign apply to like and unlike ions respectively, r_0 is the nearest-neighbor distance, η is hardness parameter and A is given by

$$A = \frac{0.29126 \left(\frac{e^2}{r_0^4} \right) \eta}{\left[\exp\left(\frac{-r_0}{\eta} \right) + 2\sqrt{2} \exp\left(\frac{-r_0\sqrt{2}}{\eta} \right) \right]} \tag{7}$$

It is assumed that the crystal is deformed homogeneously. When the crystal is deformed homogeneously, the distance between (v, o) and (u, m) ion in the deformed and non- deformed states, R_{uv}^{mo} and r_{uv}^{mo}, are related to the Lagrangian strains α_{ij} as follows

$$(R_{uv}^{mo})^2 - (r_{uv}^{mo})^2 = 2 Y_{uvi}^{mo} Y_{uvj}^{mo} \alpha_{ij} = 2 Z_{uv}^{mo} \tag{8}$$

Where Y_{uvi}^{mo} is the i-th Cartesian component of the vector r_{uv}^{mo}. The definition of the quantity Z_{uv}^{mo} is also expressed in Equation (8). The internal energy U_0 given by equation (5) can be expanded in terms of Z_{uv}^{mo}, which will yield quadratic, cubic and quartic terms as given below:

$$U_2 = \frac{1}{2V_c} \sum{}' [Z^2 D^2 Q(R)/2!]_{R=r}$$

$$= \frac{1}{4V_c} [\alpha_{ij}\alpha_{kl} \sum{}' Y_i Y_j Y_k Y_l D^2 Q(R)]_{R=r}$$

$$U_3 = \frac{1}{2V_c} \sum{}' [Z^3 D^3 Q(R)/3!]_{R=r}$$

$$= \frac{1}{12V_c}[\alpha_{ij}\alpha_{kl}\alpha_{mn}\sum{}'Y_iY_jY_kY_lY_mY_nD^3Q(R)]_{R=r}$$

$$U_4 = \frac{1}{2V_c}\sum{}'[Z^4D^4Q(R)/4!]_{R=r}$$

$$= \frac{1}{48V_c}[\alpha_{ij}\alpha_{kl}\alpha_{mn}\alpha_{pq}\sum{}'Y_iY_jY_kY_lY_mY_nY_pY_qD^4Q(R)]_{R=r} \tag{9}$$

Where $\quad D = \dfrac{d}{RdR}$

With reference to Equations (3) and (4) and comparison of Equations (1) and (9), one may obtain the static elastic constants which are presented in Table 2.1. For a central force model, there are only two independent SOECs, three independent TOECs and four independent FOECs at absolute zero temperature. As in the case of the internal energy U_0, the vibrational free energy is also expanded in terms of strains, the quadratic, cubic and quartic terms are as below:

$$U_2 = \left[\frac{1}{V_c\,2!}\right]\sum{}'\sum{}'[Z'Z(D'D)U^{vib}]_{Z=0}$$

$$= \left[\frac{1}{2V_c}\right]\alpha_{ij}\alpha_{kl}\,f_{ijkl}$$

$$U_3 = \left[\frac{1}{V_c\,3!}\right]\sum{}'\sum{}'\sum{}'[Z'Z''Z(D'D''D)U^{vib}]_{Z=0}$$

$$= \left[\frac{1}{6V_c}\right]\alpha_{ij}\alpha_{kl}\alpha_{mn}\,f_{ijklmn}$$

$$U_4 = \left[\frac{1}{V_c\,4!}\right]\sum{}'\sum{}'\sum{}'\sum{}'[Z'Z''Z'''Z(D'D''D'''D)U^{vib}]_{Z=0}$$

$$= \left[\frac{1}{24V_c}\right]\alpha_{ij}\alpha_{kl}\alpha_{mn}\alpha_{pq}\,f_{ijklmnpq} \tag{10}$$

Where $\quad f_{ijkl} = \sum{}'\sum{}'[Y_iY_jY_k'Y_l'(D'D)U^{vib}]_{R=r}, \qquad f_{ijklmn} = \sum{}'\sum{}'\sum{}'[Y_iY_jY_k'Y_l'Y_m''Y_n''(D''D'D)U^{vib}]_{R=r}$

and $\quad f_{ijklmnpq} = \sum{}'\sum{}'\sum{}'\sum{}'[Y_iY_jY_k'Y_l'Y_m''Y_n''Y_p'''Y_q'''(D'''D''D'D)U^{vib}]_{R=r}$

On comparison Equations (1) and (10); one determines the vibrational elastic constants.

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 50K 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 Figures 1 – 12.

RESULTS AND DISCUSSIONS

The SOECs, TOECs and FOECs in 10^{10} N/m^2 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 of the SOECs in 10^{-9} m^2/N and Partial Contractions in 10^{12} N/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 CoO are represented graphically in Fig 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].

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 Figure 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 Figure 2 and the variation of C_{144}, C_{166} and C_{456} are given in Figure 3. There are eleven 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 all these are given in Figures 4 - 7. 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_{112}/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 and TOECs are given in Figures 8 - 10. 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 Figure 11. 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 Figure 12. 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.

ACKNOWLEDGEMENT

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Table 1. The nearest neighbour distance (r_0) and hardness parameter (q) in 10^{-10} m and SOECs in 10^{10} N/m^2 for TeO crystal at room temperature.

Melting Point (K)	r_0	q	C_{11}	C_{12}	C_{44}	Ref.
643	2.7865	0.345	20.711	22.109	22.346	Present

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

C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	Ref.
-234.110	-102.256	33.826	32.482	-88.531	31.679	Present

Table 3. The FOECs in 10^{10} N/m^2 for TeO 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}
2392.0	301.0	434.1	-77.23	-74.48	387.4	-79.45	447.1	-74.01	452.6	-74.41

Table 4. The FOPDs of SOECs and TOECs for TeO crystal at room temperature.

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

Table 5. The SOPDs of SOECs in 10^{-9} m^2/N and partial contractions in 10^{12} N/m^2 for TeO crystal at room temperature.

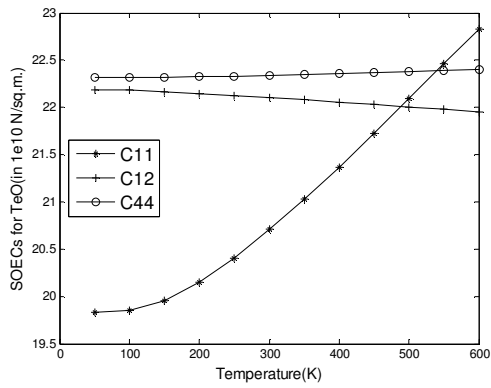| $\dfrac{d^2C_{11}}{dP^2}$	$\dfrac{d^2C_{12}}{dP^2}$	$\dfrac{d^2C_{44}}{dP^2}$	W_{11}	W_{12}	W_{44}
0.380	0.124	0.110	43.101	10.842	12.728

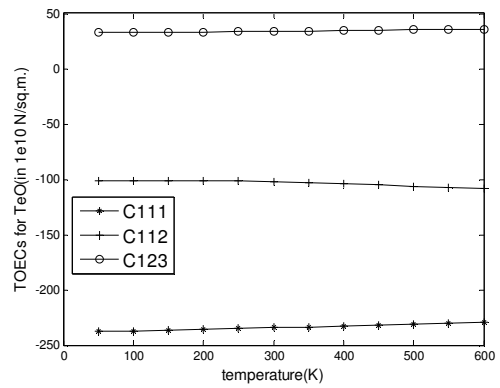Figure 1 Temp. Variation of SOECs for TeO
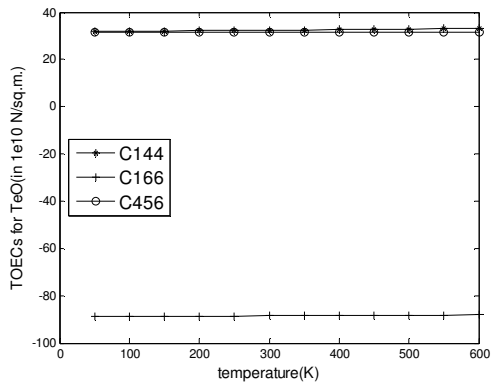

Figure 2 Temp. Variation of TOECs for TeO

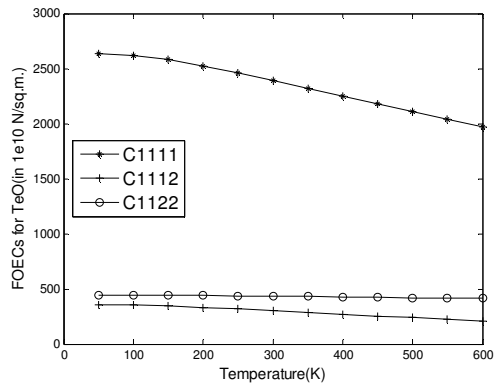Figure 3 Temp. Variation of TOECs for TeO
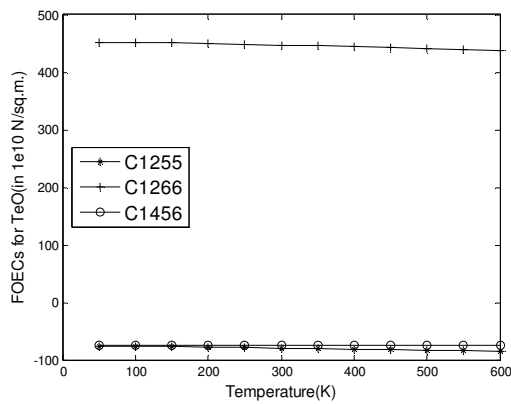

Figure 4 Temp. Variation of FOECs for TeO

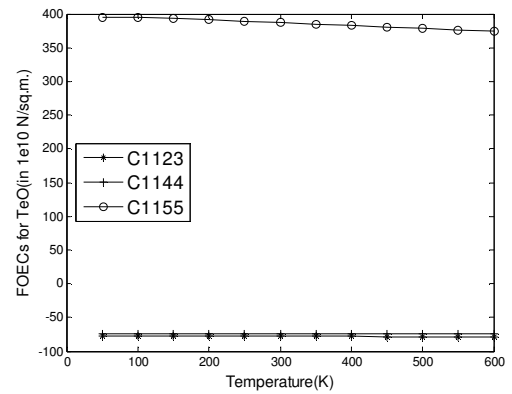Figure 5. Temp. Variation of FOECs for TeO
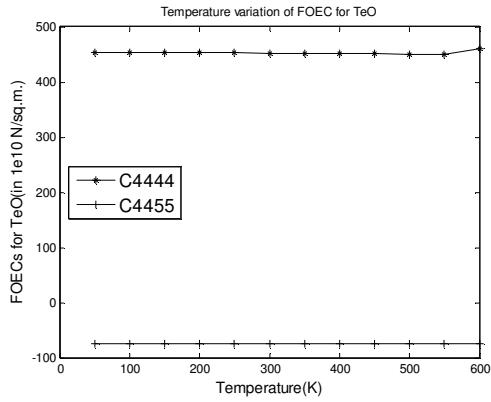

Figure 6 Temp. Variation of FOECs for TeO
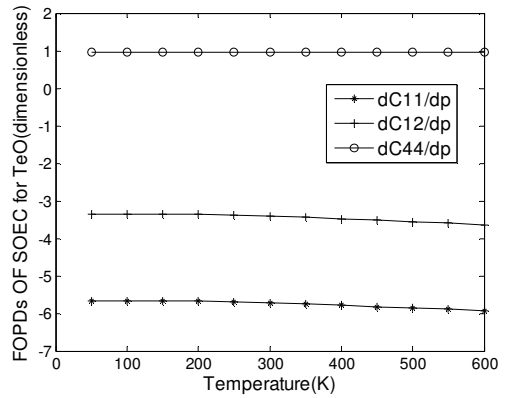
Figure 7 Temp. Variation of FOECs for TeO

Figure 8 Temp. Variation of FOPDs of SOECs for TeO

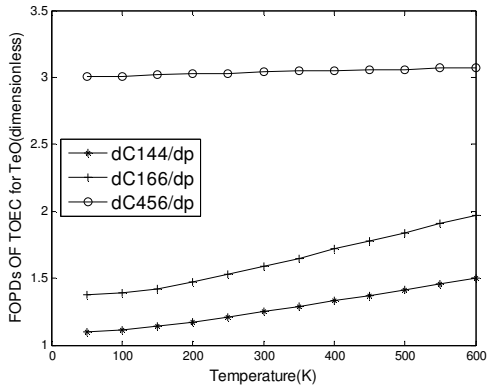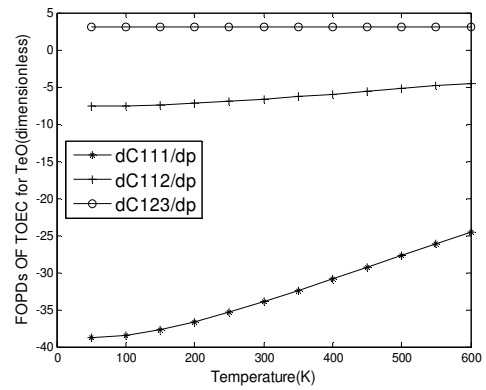Figure 9 Temp. Variation of FOPDs of TOECs for TeO

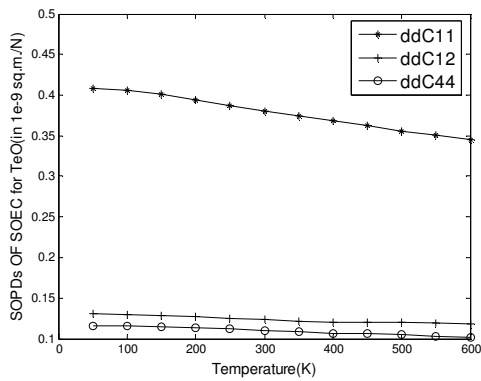Figure 10 Temp. Variation of FOPDs of TOECs for TeO
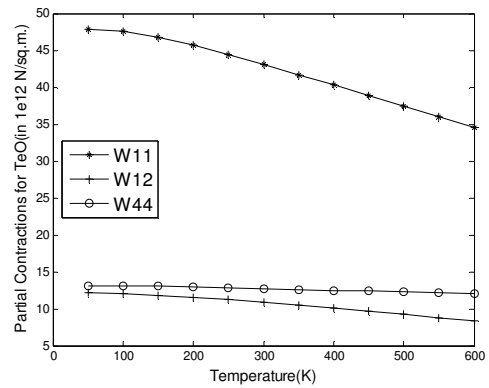

Figure 11 Temp. Variation of SOPDs of SOECs for TeO

Figure 12 Temp. Variation of partial contractions for TeO