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Comparative Study of Anharmonic Properties of Oxides Having Face Centered Cubic Crystal Structure of Second and Third Order

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Abstract: *A theory has been evolved for obtaining anharmonic properties of oxides having face centered cubic crystal symmetry using long-range Coulomb and short-range Born-Mayer potentials starting from the nearest-neighbour distance and hardness parameter. The second order elastic constants are obtained for oxides of Cd, Co, Fe, Nb, Ni, Te, Ti and Zr at elevated temperature. The room temperature data are utilized for obtaining the first order pressure derivatives of second order elastic constants, the second order pressure derivatives of second order elastic constants and partial contractions of these oxides. The results are presented and discussed.*

Keywords: Centered Cubic Crystal

I. INTRODUCTION

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 order elastic constants (SOECs) . When the values of these elastic constants of crystals can be treated within the limit of the continuum approximation in a quantitative manner. Various cystal anharmonicities such as thermal expansion, specific heat at higher temperature, temperature variation of ultrasonic velocity and attenuation, first order pressure derivatives (FOPD) of TOECs,the second order pressure derivative (SOPD) of SOECs, partial contraction and deformation of crystals under large forces, the FOECs are to be considered extensively.

In last decade, considerable interest has been taken in investigation of acoustic properties of substances [1-11]. Various investigators have enriched the field of ultrasonic by their experimental and theoretical approach. The ultrasonic now has become a subject of considerable interest due to its various applications in navy, industry, medicines, science and technology and different aspects of modern life. The ultrasonic study in materials has become an independent branch of engineering itself. The ultrasonic is now used as a versatile tool in the study of internal structure and inherent properties of crystals, surface microscopy, holographic imaging and optical data processing. Not only this, engineers are using it in non-destructive testing of industrial components and doctors for physiotherapy and diagnosis in cardiology, neurology, ophthalmology , gynaecology etc. [12-15].

Many efforts have been made in the study of elastic properties of crystals of different kinds [16-25] utilizing various physical conditions and using several techniques. Some fruitful results have been obtained by various investigators while studying the anharmonic properties of the substances possessing different crystals structures. Some have studied temperature variation of SOECs of alkali halides [16,21-22,26], of rare gas crystals [27] , of a few alkali cyanides using theoretical [16], ultrasonic [28-30] and Brillouin scattering [31] methods and of mixed alkali halides-cynides [32] . The theoretical evaluation of TOECs of a few rare gas crystals [27,33] , noble metals [17], chalcogenides [34], alkali halides [16,35], fluorite crystals [36] and tetrahedral bonded nitrides [18] have been made by some workers. Some efforts have been made for obtaining TOECs of crystals having different structure [25,37,37]. No complete experimental or theoretical efforts have been made so for in obtaining the temperature variation of SOECs, TOECs and FOECs , the FOPD of SOECs and TOECs, the SOPD of SOECs and partial contraction of crystals possessing various structures.

The present work deals with the formulation for obtaining SOECs at any temperature , the FOPD of SOECs and TOECs, SOPD of SOECs and partial contractions assuming long-range Coulomb and short-range Born-Mayer potentials starting from the nearest-neighbour

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distance and hardness parameter for crystals of cubic symmetry and which consist of divalent ions.

II. FORMULATION

The elastic strain energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as follows [38]

$$U_0 = U_2 + U_3 + U_4$$
$$= C_{ijkl}\, x_{ij}\, x_{kl}/2! + C_{ijklmn}\, x_{ij}\, x_{kl}\, x_{mn}/3! + C_{ijklmnpq}\, x_{ij}\, x_{kl}\, x_{mn}\, x_{pq}/4!$$
$$C_{11}\,(X_{11}^2 + x_{22}^2 + X_{33}^2)/2 + C_{12}\,(x_{11}x_{22} + x_{22}x_{33} + x_{33}x_{11}) + 2C_{44}\,(x_{12}^2 + x_{23}^2 + x_{31}^2)$$
$$+ C_{111}\,(x_{11}^3 + x_{22}^3 + x_{33}^3)/6$$
$$+ C_{112}\,[x_{11}^2\,(x_{22} + x_{33}) + x_{22}^2\,(x_{33} + x_{11}) + (x_{33}^2\,(x_{11} + x_{22})]/2$$
$$+ C_{123}\, x_{11}\, x_{22}\, x_{33} + 2C_{144}\,(x_{11}\, x_{23}^2 + x_{22}\, x_{31}^2 + x_{33}\, x_{12}^2)$$
$$+ 2C_{166}\,[x_{12}^2\,(x_{11} + x_{22}) + x_{23}^2\,(x_{22} + x_{33}) + x_{31}^2\,(x_{33} + x_{11})]$$
$$+ 8C_{456}\, x_{12}\, x_{23}\, x_{31} + C_{1111}\,(x_{11}^4\, x_{22}^4 + x_{33}^4)/24$$
$$+ C_{1112}\,[x_{11}^3\,(x_{22} + x_{33}) + (x_{22}^3\,(x_{33} + x_{11}) + x_{33}^3\,(x_{11} + x_{22})]/6$$
$$+ C_{1122}\,(x_{11}^2\, x_{22}^2 + x_{22}^2\, x_{33}^2 + x_{33}^2\, x_{11}^2)/4$$
$$+ C_{1123}\, x_{11}\, x_{22}\, x_{33}\,(x_{11} + x_{22} + x_{33})/2$$
$$+C_{1144}\,(x_{11}^2\, x_{23}^2 + x_{22}^2\, x_{31}^2 + x_{33}^2\, x_{12}^2)$$
$$+C_{1155}\,(x_{11}^2\,(x_{31}^2 + x_{12}^2) + x_{22}^2\,(x_{12}^2\, x_{23}^2\,(x_{23}^2\, x_{312})]$$
$$+2C_{1255}\,(x_{11}\, x_{22}\,(x_{23}^2 + x_{31}^2) + x_{22}\, x_{33}\,(x_{31}^2 + x_{12}^2) + x_{33}\, x_{11}\,(x_{12}^2 + x_{23}^2)] \quad (1)$$
$$+ 2C_{1266}\,(x_{11}\, x_{22}\, x_{12}^2 + x_{22}\, x_{23}\, x_{23}^2 + x_{33}\, x_{11}\, x_{31}^2)$$
$$+8C_{1456}\, x_{12}\, x_{23}\, x_{31}\,(x_{11} + x_{22} + x_{33}) + 2C_{4444}\,(x_{12}^4 + x_{23}^4 + x_{31}^4)/3 + 4C_{4455}\,(x_{12}^2\, x_{23}^2 + x_{23}^2\, x_{31}^2 + x_{31}^2\, x_{12}^2)$$

Where C_{ijkl} , C_{ijklmn} and $C_{ijklmnpq}$ are SOEC , TOEC and FOEC in tensorial form , x_{ij} are the Lagrangian strain components, C_{IJ} , C_{IJK} and C_{IJKL} are SOECs, TOECs, FOECs in Brugger's definition [39] and Voigt notations

Expressions for the Third and Fourth order elastic constants at 0K for oxides having F.C.C. crystal structure.

$C_{111}^0 = 41.0556\ G - G_3 - 2G_4$
$C_{112}^0 = C_{166}^0 = 4.8345\ G - G_4$
$C_{123}^0 = C_{144}^0 = C_{456}^0 = 2.7135\ G$
$C_{1111}^0 = -322.8582\ G + G_5 + 2G_6$
$C_{1112}^0 = C_{1155}^0 = 17.7282\ G + G_6$
$C_{1122}^0 = C_{1266}^0 = C_{4444}^0 = 22.4637\ G + G_6$
$C_{1123}^0 = C_{1144}^0 = C_{1255}^0 = C_{1456}^0 = C_{4455}^0 = -6.3399\ G$

Where;

$G = e^2/r_0^4$
$G_3 = (3/r_0^2 + 3/qr_0 + 1/q^2)\, Q(r_0)/q$
$G_4 = (3\sqrt{2}/r_0^2 + 6/qr_0 + 2\sqrt{2}/q^2)\, Q(r_0\sqrt{2})/4q$
$G_5 = (15/r_0^3 + 15/qr_0^2 + 6/q^2r_0 + 1/q^3)\, r_0\, Q(r_0)/q$
$G_6 = (15\sqrt{2}/4r_0^3 + 15/2qr_0^2 + 3\sqrt{2}/q^2r_0 + 1/q^3)\, r_0\, Q(r_0\sqrt{2})/2q$

Expressions for vibrational contribution to the Third and Fourth order elastic constants for oxides having F.C.C. crystal structure.

$C_{111}^{vib} = f_3F_1^3 + f_2F_2F_1 + f_1F_3$
$C_{112}^{vib} = f_1F_1^3 + f_2F_1(2F_5 + F_2) + f_1F_6$
$C_{123}^{vib} + f_3F_1^3 + 3f_2F_1F_5$
$C_{144}^{vib} = f_2F_1F_5$
$C_{166}^{vib} = f_2F_1F_5 + f_1F_6$
$C_{456}^{vib} = 0$
$C_{1111}^{vib} = f_4F_1^4 + 6f_3F_1^2F_2 + 3f_2F_2^2 + 4f_2F_1F_3 + f_1F_4$

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$C_{1456}^{vib} = 0$
$C_{1112}^{vib} = f_4F_1^4 + 3f_3F_1^2(F_5 + F_2) + 3f_2F_5F_2 + f_2F_1(3F_6 + F_3) + f_1F_7$
$C_{1122}^{vib} = f_4F_1^4 + 2f_3F_1^2(2F_5 + F_2) + f_2(2F_5^2 + F_2^2) + 4f_2F_1F_2 + f_1F_7$
$C_{1123}^{vib} = f_4F_1^4 + f_3F_1^2(5F_5 + F_2) + f_2F_1(2F_5 + F_2) + 2f_2F_1F_6$
$C_{1144}^{vib} = f_3F_1^2F_5 + f_2F_5F_2$
$C_{4444}^{vib} = 3f_2F_5^2 + f_2F_7$
$C_{1155}^{vib} = f_3F_1^2F_5 + f_2F_5F_2 + 2f_2F_1F_6 + f_1F_7$
$C_{4455}^{vib} = f_2F_5^2$
$C_{1255}^{vib} = f_3F_1^2F_5 + f_2F_5^2 + f_2F_1F_6$
$C_{1266}^{vib} = f_3F_1^2F_5 + f_2F_5^2 + 2f_2F_1F_6 + f_1F_7$

Expressions for f_n for oxides having F.C.C. crystal structure..
$f_1 = {}_{f0}S;$
$f_2 = f_0[(X/S_1) + S]/2;$
$f_3 = f_0[(2X^2S/3S_1) + (X/S_1) + S]/48;$
$f_4 = -f_0[(X^3S^2/3S_1) + (X^3/6S_1^2) + (X^2S/S_1) + (5X/4S_1) + (5S/4)]/144;$

Expression for F_n for oxides having F.C.C. crystal structure.
$F_0 = 1/[(q_0-2)(Q(r_0) + 2(q_0-\sqrt{2})Q(r_0\sqrt{2})]$
$F_1 = 2[(2 + 2q_0-q_0^2)Q(r_0) + 2(\sqrt{2} + 2q_0-\sqrt{2}q_0^2)Q(r_0\sqrt{2})]F_0;$
$F_2 = 2(-6 - 6q_0-q_0^2 + q_0^3)Q(r_0)F_0 + F_5;$
$F_3 = 2(30 + 30q_0 + 9q_0^2 - q_0^3q_0^4)Q(r_0)F_0 + F_6;$
$F_5 = (-3\sqrt{2} - 6q_0 - \sqrt{2}q_0^2 + 2q_0^3)Q(r_0\sqrt{2})F;$
$F_6 = [(15/\sqrt{2}) + 15q_0 - (9/\sqrt{2})q_0^2 - q_0^3 - \sqrt{2}q_0^4]Q(r_0\sqrt{2})F_0;$

Expressions for the First order pressure derivatives of the Third elastic constants for oxides having F.C.C. crystal structure.
$dc_{111}/dP = -(-3C_Q + 3C_{111} + C_{1111} + 2C_{1112})C_0;$
$dc_{112}/dP = -(C_Q + 3C_{112} + C_{1112} + C_{1122} + C_{1123})C_0;$
$dc_{123}/dP = -(-C_Q + 3C_{123} + 3C_{1123})C_0;$
$dc_{144}/dP = -(C_Q + 3C_{144} + C_{1144} + 2C_{1244})C_0;$
$dc_{166}/dP = -(-C_Q + 3C_{166} + C_{1166} + 2C_{1244})C_0;$
$dc_{456}/dP = -(-C_Q + 3C_{456} + 3C_{1456})C_0;$

III. EVALUATION

A brief account of formulation is given in Section 2 and the expressions are tabulated in Tables I-VI. The different computer programs needed for present work are written, feeded and executed for oxides of Cd, Co, Fe, Ne, Ni, Te, Ti and Zr. Using the concept of nearest-neighbour distance [43,48] and hardness parameter [34,49-51], the SOECs , TOECs and FOECs for oxides of Cd, Co, Fe, Nb, Ni, Te, Ti and Zr are evaluated at 0K using Table I and the resulting

IV. DISCUSSION

It is obvious from Table VII that there are two independent SOECs, three independent TOECs and four independent FOECs of oxides of Cd, Co, Fe, Nb, Ni,Te,Ti and Zr at 0K and are of the order of 10^{10} Newton/meter^2 . C_{12}^0 is higher than C_{11}^0 exceptCdO in which both are approximately equal and both elastic constants are positive in nature. C_{111}^0 and C_{112}^0 are of the same order and negative in nature and C_{123}^0 is positive in nature and is less than half of the absolute value of C_{112}^0. C_{1123}^0 is greater than C_{1112}^0 and C_{1112}^0 is greater than C_{1122}^0. C_{1111}^0 is larger than remaining FOECs and is about nine times. The natural frequency ω_0 for CdO , CoO, FeO, NbO, NiO , TeO, TiO and ZrO (Table VIII) is of the

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order of 10^{13}/second . The temperature coefficients (Table VIII) F_1 , F_4 and F_5 are negative in nature and remaining others are positive in nature. The absolute values of Fn's are in the following order:

$$F_5 > F_6 > F_7 > F_3 > F_4 > F_1 > F_2$$

There are three independent SOECs of oxides of Cd, Co, Fe, Nb, Ni,Te,Ti and Zr at room temperature (Table IX) . All SOECs are positive in nature . C_{11} is less than C_{12} and C_{44} except for CdO in which all are equal approximately . One may say that C_{11} is less than remaining SOECs for these oxides . One may see from Table IX that there are six independent TOECs at elevated temperature which are of the order of 10^{12} Newton/meter^2 . C_{123} , C_{144} and C_{456} are positive in nature and remaining others are negative in nature . C_{123} , C_{144} and C_{456} are of the same order and are approximately equal . C_{112} and C_{166} are of the same order and approximately equal . The absolute value of C_{111} is higher than remaining others . The absolute value of TOECs follows the following sequence :

$$C_{111} > C_{166} > C_{112} > C_{144} > C_{456} > C_{123}$$

So far as the matter is concered with FOECs (Table X), one obtains a set of eleven independent FOECs at room temperature. Some of them sre positive in nature and remaining others are negative in nature . C_{1111} shows dual nature . It is positive for CdO , TeO and ZrO and is negative for other oxides . One may write the absolute values of FOECs in the following order:

$$C_{1123} > C_{1112} > C_{1122} > C_{1111} > C_{4444} > C_{1266} >$$
$$C_{1155} > C_{1144} > C_{1255} > C_{4455} > C_{1456}$$

Substance	C^0_{111}	C^0_{112}	C^0_{123}	C^0_{1111}	C^0_{1112}	C^0_{1122}	C^0_{1123}
CdO	-248.74	-74.346	26.807	3045.6	341.58	332.88	388.37
CoO	-214.44	-107.57	38.324	2558.3	481.37	461.98	548.26
FeO	-212.71	-108.85	38.769	2536.2	486.67	466.76	554.33
NbO	-206.83	-113.05	40.234	2461.9	504.03	482.34	574.25
NiO	-183.05	-128.47	45.629	2171.7	567.31	538.39	646.94
TeO	-236.35	-88.562	31.722	2860.3	401.96	389.42	457.32
TiO	-199.74	-117.88	41.922	2373.8	523.94	500.09	597.10
ZrO	-237.52	-87.887	31.488	2869.9	399.12	386.78	454.07

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