Ultrasonic Properties of Sodium Halides Crystals

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ABSTRACT

Elastic constant of solid can be used to illustrate the linear and non-linear mechanical and dynamical behaviour of crystals which provide the crucial information about the nature of longand short-range potentials. In this paper, we have discussed the Ultrasonic properties of ionic crystals such as NaCl, NaBr, NaI, NaF. These elastic constants are estimate using Coulomb and Börn-Mayer type interaction potential with two primary physical parameters ie. nearest neighbour distance and hardness parameter at elevated temperatures. Later on, ultrasonic velocity and various ultrasonic physical quantities ie. average Grüneisen number, specific heat, phonon-velocity, thermal relaxation point, non-linear properties are calculated at different temperatures. The outcomes hence got are contrasted with experimental data and found in well concurrence with current data.

INTRODUCTION

The elastic energy density for a crystal can be expressed as a higher series of strain using Taylor's series expansion[1,2]. The second order elastic constants (SOECs), third order elastic constants (TOECs) and fourth order elastic constants (EOECs) are the coefficients of quadratic, cubic and quartic terms. Researcher can find out various properties of the solid by knowing the information of these elastic constants. Various ultrasonic properties of solids like specific heat at elevated temperature, thermal expansion, temperature dependency of ultrasonic velocity & attenuation, first order pressure dependence of second order elastic constants, temperature dependence of second order elastic constants and Grüneisen number are directly related to second and third order elastic constants[3-5]. In the last year some fruitful researches are done by different researchers during the study of ultrasonic properties of various crystal structures. A study was reported for obtaining the ultrasonic behaviour of different oxides [6-9]. Some investigators have computed anisotropic elastic constants of a B_2 structured iron aluminide (FeAl) alloy at different temperatures using Coulomb and Börn Mayer model [10,11]. Few researchers reported some results on the ultrasonic

behaviour of different oxides in the temperature range of 300 to 500K using ultrasonic techniques [12-15]. Investigation have also been made on temperature dependent ultrasonic velocities & ultrasonic Grüneisen parameter in BkX (XN, P, As, Sb) in the temperature range 100-500K along the <100>, <110> and <111> for longitudinal and shear modes of propagation for the same evaluation[16,17]. a study of the elastic behaviour of different sedimentary rocks has also been developed[18].

In present investigations, some efforts have been made for obtaining the second, third and fourth order elastic constants, the first order pressure derivatives of the second and third order elastic constants, the second order pressure derivatives of the second order elastic constants and partial contractions of divalent crystals having face centred cubic crystals starting from nearest neighbour distance and hardness parameter utilizing the Coulomb and Börn-Mayer potentials. In this work, a study has been made for obtaining the ultrasonic properties of different crystals such as sodium halides (NaCl, NaBr, NaI, NaF) at different temperatures[19-22]. The achieved results are discussed that provides valuable information about the chosen materials.

FORMULATION

The elastic strain energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as follows [23];

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

$x_{33}\, x_{11}\, (x_{12}^2 + x_{23}^2)]$

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

$+ 8C_{1456}\, x_{12}\, x_{23}\, x_{31}\, (x_{11} + x_{22} + x_{33}) + 2/3\, .\, C_{4444}\, (x_{12}^4$

$+ x_{23}^4 + x_{31}^4) + 4C_{4455}\, (x_{12}^2\, x_{23}^2 + x_{23}^2\, x_{31}^2 + x_{31}^2\, x_{12}^2)$ (1)

Where C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$ are second, third and fourth order elastic constants in tensorial form, x_{ij} are the Lagrangian Strain components, C_{IJ}, C_{IJK} and C_{IJKL} are the second, third and fourth order elastic constants in Brugger's definition [24] and Voigt notations.

The elastic constants of the second, third and fourth order are defined as [25];

$$C_{ijkl} = C_{IJ} = (\partial^2 U/\partial x_{ij}\, \partial x_{kl})_{x=0}$$

$$C_{ijklmn} = C_{IJK} = (\partial^3 U/\partial x_{ij}\, \partial x_{mn}\, \partial x_{kl})_{x=0}$$

and

$$C_{ijklmnpq} = C_{IJKL} = (\partial^4 U/\partial x_{ij}\, \partial x_{kl}\, \partial x_{mn}\, \partial x_{pq})_{x=0} \quad (2)$$

The free charge density [18,19] of a crystal at a finite temperature T is

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

$$U^{vib} = KT/NV_c\, \Sigma^{3sN}_{i=1} \text{In } 2 \text{ Sinh } (h\omega_i/KT) \quad (3)$$

Where U_0 is the internal energy per unit volume of the crystal when all ions are at rest on their lattice points, U^{vib} 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 can be separated into two parts

$$C_{IJ} = C^0_{IJ} + C_{IJ}^{vib}$$

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

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

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 "O" 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;

$$U_0 = 1/2V_c\, .\, \Sigma^{s}_{v=1} \Sigma\, Q_{uv}\, (R_{uv}^{mo}) = \Sigma\, Quv(R)/2V_c \quad (5)$$

$$m \neq o$$

$$u \neq v$$

Where R^{mo}_{uv} is the distance between the v-th ion in the oth cell and the u-th ion in the m-th cell and Quv is the interaction potential between the ions. The indices (v,o) and (u,m) are sometimes dropped when no confusion occurs. One assumes that Quv is the sum of the Coulomb and the Born-Mayer [26] potentials.

$$Quv(R) = \pm (e^2/R) + A \exp(-R/q) \quad (6)$$

Where e is the electric charge, ± sign apply to like and unlike ions, respectively and A and q are some parameters.

One further assumes that A and q are the same for all short-range interactions, where q is the repulsive parameter of the crystal and A is given by

$$A = -0.29126q\,(e^2/r_0^4)/[\exp(-r_0/q) + 2\sqrt{2}\exp(-r_0\sqrt{2}/q)] \quad (7)$$

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 x_{ij} as follows

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

Where Y_{uvi}^{mo} is the i-th cortesian component of the vector r^{mo}_{uv}. The definition of the quantity Z_{uv}^{mo} is also expressed in equation (8). The internal energy Uo given by equation (5) can be expanded in terms of Z, which yields quadratic, cubic and quartic terms as shown below

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

$$= 1/4V_c \,.\, [x_{ij}\, x_{kl} \sum' Y_I\, Y_j\, Y_k\, Y_l\, D^2Q(R)_{R=r}$$

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

$$= 1/12V_c \,.\, [x_{ij}\, x_{kl}\, x_{mn} \sum' Y_I\, Y_j\, Y_k\, Y_l\, Y_m\, Y_n\, D^3Q(R)]_{R=r}$$

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

$$= 1/48V_c \,.\, [x_{ij}\, x_{kl}\, x_{mn}\, x_{pq} \sum' Y_IY_jY_kY_lY_mY_nY_pY_qD^4Q(R)]_{R=r} \quad (9)$$

With the abbreviation D = d/(RdR) with reference to Equations (3) and (4) and comparison of Equations (1) and (9), one obtains the static elastic constants which are shown in Table I. For a central force model, there are only two independent SOECs, three independent TOECs and four independent FOECs at 0K. 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

$$U_2 = 1/V_c2! \,.\, \sum' \sum' [Z'\,Z\,(D'\,D)U^{vib}]_{Z=0}$$

$$= 1/2V_c\, x_{ij}\, x_{kl}\, f_{ijkl}$$

$$U_3 = 1/V_c3! \,.\, \sum' \sum' \sum' [Z'\,Z''\,Z\,(D'\,D''\,D)U^{vib}]_{Z=0}$$

$$= 1/6V_c\, x_{ij}\, x_{kl}\, x_{mn}\, f_{ijklmn}$$

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

$= 1/24V_c \, x_{ij} \, x_{kl} \, x_{mn} \, x_{pq} \, f_{ijklmnpq}$ (10)

Where;

$Fijkl = \sum' \sum' [Y_I \, Y_j \, Y_k' \, Y_l' \, (D' \, D) \, U^{vib}]_{R=r}$

$Fijklmn = \sum' \sum' \sum' [Y_I \, Y_j \, Y_k' \, Y_l' \, Y''_m \, Y''_n (D'' \, D' \, D) \, U^{vib}]_{R=r}$

and

$Fijklmnpq = \sum' \sum' \sum' \sum' [Y_i \, Y_j \, Y'_k \, Y'_l \, Y''_m \, Y''_n \, Y'''_p \, Y'''_q (D''' \, D'' \, D' \, D) \, U^{vib}]_{R=r}$

Here the abbreviations $Z_{u'v'}^{m'o} \rightarrow Z'$ $[d/\{R_{u'v'}^{m'o} \, dR_{u'v'}^{m'o}\}] \rightarrow D'$, etc. are used and by comparing Equations (1) and (10), one can determine the vibrational elastic constants. These are given in Table II. These are shown as a combination of g_n and F_n which are evaluated conveniently by taking crystals symmetry [27] into account and the expressions for g_n and F_n are shown in Tables III & IV. By adding the vibrational elastic constants to the static elastic constants, one may get SOECs, TOECs and FOECs at any temperature.

The first order pressure derivatives of SOECs are related to SOECs and TOECs, the first order pressure derivatives of TOECs and second order pressure derivatives of SOECs are concerned with SOECs, TOECs and FOECs and partial contractions are mere combination of FOECs. The expressions for the first and second order pressure derivatives of SOECs and the first order pressure derivatives of TOECs [28,29], partial contractions for alkali cyanides [31,32] are given in Tables V&VI.

Table I

Expressions for the Second, Third and Fourth Order Elastic constants at 0K for SnSe, SnTe and BiTe.

$C^0_{11} = -6.27732G + G_1 + 2G_2$

$C^0_{12} = C^0_{44} = 1.3911 \, G + G_2$

$C^0_{111} = 41.0556G - G_3 - 2G_4$

$C^0_{112} = C^0_{166} = 4.8345G - G_4$

$C^0_{123} = C^0_{144} = C^0_{456} = 2.7135 \, G$

$C^0_{1111} = -322.8582G + G_5 + 2G_6$

$C^0_{1112} = C_{1155} = 17.7282G + G_6$

$C^0_{1122} = C^0_{1266} = C^0_{4444} = 22.4637G + G_6$

$C^0_{1123} = C^0_{1144} = C^0_{1255} = C^0_{1456} = C^0_{4455} = -6.3399G$

Where;

$G = e^2/r_0^4$

$G_1 = (1/r_0 + 1/q)\, Q(r_0)/qr_0$

$G_2 = (\sqrt{2}/2r_0 + 1/q)\, Q(r_0\sqrt{2})/qr_0$

$G_3 = (3/r_0^2 + 3/qr_0 + 1/q^2)\, Q(r_0)/q$

$G_4 = (3\sqrt{2}/r_0^2 + 6/qr_0 + 2\sqrt{2}/q^2)\, Q(r_0\sqrt{2})/4q$

$G_5 = (15/r_0^3 + 15/qr_0^2 + 6/q^2 r_0 + 1/q^3)r_0 Q(r_0)/q$

$G_6 = (15\sqrt{2}/4r_0^3 + 15\ 2qr_0^2 + 3\sqrt{2}/q^2 r_0 + 1/q^3)r_0 Q$
$(r_0\sqrt{2})/$

Table II

Expressions for Vibrational Contribution to the Second,Third and Fourth Order Elastic Constants for SnSe, SnTe and BiTe.

$C_{11}^{vib} = f_1F_1^2 + f_1F_2$

$C_{12}^{vib} = f_2F_1^2 + f_1F_5$

$C_{44}^{vib} = f_1F_5$

$C_{111}^{vib} = f_3F_1^3 + f_2F_2F_1 + f_1F_3$

$C_{112}^{vib} = f_1F_1^3 + f_2F_1(2F_5 + F_2) + f_1F_6$

$C_{123}^{vib} = f_3F_1^3 + 3\, f_2\, F_1F_5$

$C_{144}^{vib} = f_2F_1F_5$

$C_{166}^{vib} = f_2F_1F_5 + f_1F_6$

$C_{456}^{vib} = 0$

$C_{1111}^{vib} = f_4F_1^4 + 6f_3\, F_1^2\, F_2 + 3f_2F_2^2 + 4f_2F_1F_3 + f_1F_4$

$C_{1456}^{vib} = 0$

$C_{1112}^{vib} = f_4F_1^4 + 3f_3\, F_1^2\, (F_5 + F_2) + 3f_2F_5F_2 + f_2F_1(3F_6 + F_3)$
$+ f_1F_7$

$C_{1122}^{vib} = f_4F_1^4 + 2f_3\, F_1^2\, (2F_5 + F_2) + f_2\, (2F_5^2 + F_2^2) + 4f_2F_1F_2$
$+ f_1F_7$

$C_{1123}^{vib} = f_4F_1^4 + f_3\, F_1^2\, (5F_5 + F_2) + f_2\, F_1(2F_5 + F_2 + 2f_2F_1F_6$

$C_{1144}^{vib} = f_3F_1^2F_5 + f_2\, F_5F_2$

$C_{4444}^{vib} = 3f_3F_5^2 + f_2\, F_7$

$C_{1155}^{vib} = f_3F_1^2F_5 + f_2\, F_5F_2 + 2f_2F_1F_6 + f_1F_7$

$C_{4455}^{vib} = f_2F_5^2$

$C_{1255}^{vib} = f_3F_1^2F_5 + f_2\, F_5F_2 + f_2F_1F_6$

$C_{1266}^{vib} = f_3F_1^2F_5 + f_2\, F_5^2 + 2f_2F_1F_6 + f_1F_7$

Table III

Expressions for f_n for SnSe, SnTe and BiTe.

$f_1 = f_0 S;$

$f_2 = f_0[(X/S_1) + S]/2;$

$f_0 = h\omega_0/8r_0^3;$

$f_3 = f_0[(2X^2 S/3S_1) + (X/S_1) + S]/48;$

$X = h\omega_0 / KT;$

$f_4 = -f_0 [(X^3S^2/3S_1) + (X^3/6S_1^2) + (X^2S/S_1) + (5X/4S_1) + (5S/4)]/144;$

$\omega_0 = (1/M^+ + 1/M^-)/qr_0F_0;$

$S = \text{Coth } X; \quad S_1 = \text{Sin } h^2 X.$

Table IV

Expressions for F_n for SnSe, SnTe and BiTe.

$F_0 = 1/[(q_0 - 2)(Q(r_0) + 2(q_0 - \sqrt{2})Q(r_0\sqrt{2})$

$q_0 = r_0/q;$

$F_1 = 2[(2+ 2q_0 - q_0^2)Q(r_0)+ 2(\sqrt{2} + 2q_0 - \sqrt{2}\, q_0^2)Q(r_0\sqrt{2})]F_0;$

$F_2 = 2(- 6 - 6q_0 - q_0^2 + q_0^3) Q(r_0) F_0 + F_5;$

$F_3 = 2(- 30 - 30q_0 - 9q_0^2 + q_0^3 - q_0^4) Q(r_0) F_0 + F_6;$

$F_4 = 2(-210 - 210q_0 - 75q_0^2 + 5q_0^3 + 4q_0^4 + q_0^5)Q(r_0)F_0 + F_7;$

$F_5 = (- 3\sqrt{2} - 6q_0 - \sqrt{2}\, q_0^2 + 2q_0^3)Q(r_0\sqrt{2})F_0;$

$F_6 = [(15/\sqrt{2}) + 15q_0 - (9/\sqrt{2})q_0^2 - q0_0^3 - \sqrt{2}q_0^4] Q(r_0\sqrt{2}) F_0;$

$F_7 = [(105/ 2\sqrt{2}) - 105/2)q_0 - (75/ 2\sqrt{2})q_0^2 - (5/2)q_0^3 + 2\sqrt{2}\, q_0^4 + q_0^5]Q(r_0\sqrt{2}) F_0;$

Table V

Expressions for the First Order Pressure Derivatives of the Second and Third Order Elastic Constants for SnSe, SnTe and BiTe.

$dC_{11}/dP = (C_{11} + Q_Q + C_{111} + C_{112})\, C_0;$

$C_Q = C_{11} + 2C_{12}$

$dC_{12}/dP = -(-C_{11} + C_{12} + C_{123} + 2C_{112})\, C_0;$

$C_0 = 1/C_Q;$

$dC_{44}/dP = -(C_Q + C_{44} + C_{144} + 2C_{166})\, C_0;$

$dC_{111}/dP = -(-3C_Q + 3C_{111} + C_{1111} + 2C_{1112})\, C_0;$

$dC_{112}/dP = -(C_Q + 3C_{112} + C_{1112} + C_{1122} + C_{1123})C_0;$

$dC_{113}/dP = -(-C_Q + 3C_{123} + 3C_{1123})C_0;$

$dC_{144}/dP = -(C_Q + 3C_{144} + C_{1144} + 2C_{1244})C_0;$

$dC_{166}/dP = -(-C_Q + 3C_{166} + C_{1166} + 2C_{1244})C_0;$

$dC_{456}/dP = -(-C_Q + 3C_{456} + 3C_{1456})C_0;$

Table VI

Expressions for the Second Order Pressure Derivatives of the Second Order Elastic Constants and expressions for Partial Contraction of the Fourth Order Elastic Constants for SnSe, SnTe and BiTe.

$d^2C_{11}/dP^2 = [(1+3C_P)C_{11} + (4+3C_P)(C_{111} + 2C_{112}) + C_{1111} + 4C_{1112} + 2C_{1122} + 2C_{1123}]\, C_0^2;$

$d^2C_{12}/dP^2 = [(1+3C_P)C_{12} + (4+3C_P)(2C_{112} + C_{123}) + 2C_{1122} + 5C_{1123}]C_0^2;$

$d^2C_{44}/dP^2 = [(1+3C_P)C_{44} + (4+3C_P)(C_{144} + 2C_{166}) + C_{1144} + 2C_{1166} + 4C_{1244} + 2C_{1266}]\, C_0^2;$

$C_P = (4C_{11} + C_{111} + 6C_{112} + 2C_{123})\, C_0$

$Y_{11} = C_{1111} + 4C_{1112} + 2C_{1122} + 2C_{1123};$

$Y_{12} = 2C_{1112} + 2C_{1122} + 5C_{1123};$

$Y_{44} = C_{1144} + 2C_{1166} + 4C_{1244} + 2C_{1266}$

Table VII

The Melting points and the SOECs and TOECs in 10^{10} Newton/m^2 at room temperature for Sodium Halides.

Crystal	Melting Point, K	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	Ref.
NaF	1203.00	9.124	3.256	3.524	-179.27	-11.589	3.012	5.018	-13.784	5.001	
		9.085a	2.698a	2.741a	-145.04b	-26.10b	2.78b	4.1b	-10.44b	0.23b	33a,34b
		10.56	2.01	2.91							35
NaCl	1089.00	4.998	1.111	1.065	-94.258	-5.078	0.789	2.875	-6.002	2.874	
		4.415a	1.116a	1.119a	-87.30	-4.12b	0.87b	0.91b	-5.42b	1.39b	33a,36b
		6.055a	1.275a	1.452a	-87.02b	5.11b	2.77b	2.45b	-6.79b	2.09b	35a,37b
NaBr	1056.00	3.652	2.012	1.632	-76.114	-4.858	0.477	2.121	-4.808	2.101	
		3.001	1.008	0.784							33
		4.912	0.200	1.000							36
NaI	985.00	3.414	1.323	0.421	-61.125	-2.502	0.199	1.389	-3.108	1.785	
		2.400	0.703	0.963							33

Table VIII:

FOECs in 10^{10} Newton/m^2 at room temperature of Sodium Halides.

Crystal	C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1155}	C_{1255}	C_{1266}	C_{1456}	C_{4444}	C_{4455}	Ref.
NaF	251.3	-1899	-1902	-2041	-12.63	60.85	-13.00	78.08	-12.54	6.451	-1.581	
	2287	85.1	91.0	-10.33	-13.5			109		110		38
NaCl	785.6	-411.6	-408.4	-464.0	-6.087	27.11	-6.716	34.78	-6.141	36.40	-6.022	
	1201	99.2	106	-4.06	-5.74			109		114		38
NaBr	758.1	-220.9	-225.3	-250.7	-4.052	21.44	-4.832	25.56	-4.001	26.77	-4.365	
	981	95.0	104	-3.00	-4.12			101		105		38
NaI	647.0	-131.9	-140.4	-157.9	-3.411	15.01	-3.744	18.11	-3.199	20.18	-3.412	
	771	100	104	-2.40	-3.06			104		112		38

Table IX:

The FOPDs and SOPDs (in 10^{-11} Newton/m^2) of the SOECs and partial contractions (in 10^{12} Newton/m^2) of Sodium Halides.

Crystal	Y_{11}	Y_{12}	Y_{44}	dC_{11}/dP	dC_{12}/dp	dC_{44}/dP	ds/dp	dk/dp	d^2C_{11}/dP	d^2C_{12}/dp	d^2C_{44}/dp	Ref.
NaF	-149.33	-171.10	-31.22	8.11	1.74	0.85	2.89	3.96	-3.01	-5.01	-1.26	
	285.4a	309a	32.1a	10.45b	1.13b	0.71b			-2.44a	-0.78a	-1.35a	
									-3.08	-0.701	-0.688	39a,41b
												42
NaCl	-24.399	-36.258	-8.001	11.02	1.36	0.08	5.01	5.23	-0.99	-3.27	-0.70	
	18.08a	34.6a	3.69a	11.10b	1.69b	0.31b			-5.50a	-1.05a	-3.74a	
									8.05	-1.7	-0.602	39a,41b
												42
NaBr	-10.045	-20.900	-4.411	11.52	1.08	0.99	4.88	5.02	-4.12	-3.74	-0.65	
	17.11a	36.5a	4.146a	11.26b	2.973b	051b			-6.07a	-1.41a	-2.00a	
									-8.17	-1.19	-1.96	39a,41b
												42
NaI	-4.00	-12.00	-2.01	10.95	1.44	0.02	3.85	5.22	-5.78	-3.00	-0.19	
	11.22a	40.32a	3.65a	09.87b	1.77b	0.43b			-7.49c	-2.99c	-6.10c	
									-12.21	-1.79b	-1.44	39a,41b
									-10.56	-1.88	-1.65	40
												42

Table X:

The nearest neighbour distance (r_0) and hardness parameter (q) (10^{-10}m) FOPDs of the TOECs at room temperature of Sodium Halides.

Crystal	r_0	Q	dC_{111}/dP	dC_{112}/dP	dC_{123}/dp	dC_{144}/dP	dC_{166}/dP	dC_{456}/dp	Ref.
NaF	2.1203	0.284	233	358	346	-1.52	117	2.05	
			-121	-8.28	2.50	10.04	0.25	2.66	39
NaCl	2.9658	0.211	44.65	149	105	-1.20	49.0	2.59	
			-140	-19.21	1.07	0.46	-5.00	2.10	39
NaBr	2.9960	0.412	-6.84	99	111	-0.99	33.7	2.19	
			-136	-22.0	1.00	0.02	-7.33	2.34	39
NaI	3.0025	0.353	-25.47	80.40	91.18	-1.73	28.37	2.03	
			-141	-30.39	1.41	0.02	-09.0	2.44	39

Table XI:

Numerical Coefficient for Sodium Halides.

Coefficient	A_1	A_2	A_3	A_4	A_5
NaF	-7.3020	0.2154	-6.7489×10^{-4}	8.9921×10^{-7}	-4.3748×10^{-10}
NaCl	-5.0012	0.5680	-7.3201×10^{-4}	8.7012×10^{-7}	-4.0220×10^{-10}
NaBr	10.0001	0.1201	-	-	-
NaI	-10.3080	0.7710	-6.5206×10^{-3}	2.0487×10^{-5}	-4.0251×10^{-8}

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