ULTRASONIC BEHAVIOUR OF POTASSIUM HALIDE CRYSTALS

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Abstract: The purpose of this paper is to study the elastic behaviour of different kinds of Alkali Halides such as KF, KCl, KBr, KI at different temperature upto their melting point and temperature-dependent ultrasonic velocities and ultrasonic Grüneisen parameter have studied in Potassium Halide crystal. We have also computed second, third and higher order elastic constant using Coulomb and Börn-Mayer potential with the help of general potential i.e. nearest neighbour distance and hardness parameter. Further parameter like Bulk Modulus, Young's Modulus, Shear Modulus etc have also been find out for the future achievement. The theory is tested for SOECs, TOECs, FOECs and correlated physical properties of potassium halide at different temperature. The study of higher order elastic constant of potassium halide crystals have been undertaken for aim of giving needed and prime information. The data of higher order elastic constants and some physical properties are in suitable concurrence with other theoretical and experimental data.

Keyword- Ultrasonics, Acoustics, elastic constants

I. Introduction

In ultrasonic material characterization, a large number of studies have published on the uses of non-destructive evaluation for various crystals and solids. Two physical quantities such as ultrasonic velocity and attenuation are the more significant parameter which is mandatory for the ultrasonic non-destructive evaluation (NDE) technique of material characterization. Elastic constant and material density is related to ultrasonic velocity[1-3]. Ultrasonic attenuation coefficient correlates numerous physical properties like Grüneisen parameter, elastic constants, thermal relaxation time, specific heat, thermal conductivity etc. Hence, under different physical conditions the material can be characterized with the familiarity of ultrasonic parameters[4-6]. Many researchers have been worked in the field of ultrasonic behaviour of different crystals and solids[7-9]. Kailash et al[10], have shown that how ultrasonic behaviour are depends on various temperatures of lanthanum (Ln) compounds. Hyunjo et al[11], have proposed the processor for determining non-linear parameter of thick solids samples. Ultrasonic studies was made for finding the non-linear properties such as second elastic constant (SOECs), third order elastic constant (TOECs) and fourth order elastic constants (FOECs). On the other hand, FOPDs are representable in the term of SOECs and TOECs, SOPDs of SOECs of several ionic crystals[12,13].

In this recent study, a formulation have been made to evaluate of higher order elastic constants like (SOECs, TOECs & FOECs) for FCC crystal at different temperature. The whole evaluation is founded on the hypothesis that FCC crystal structure of the material does not change, when temperature varies upto their melting point. Non-linear properties of solid possessing different crystal structure are directly related with primary physical parameter such as nearest neighbour distance and repulsive parameter assuming long range Coulomb and sort-range Börn Mayer potential. Ultrasonic velocity is different in any direction for a crystal and it may change from crystal to crystal. In this paper mainly focused on the study of higher order elastic constants and non-linear properties of potassium halide (KF, KCl, KBr & KI) crystals are evaluated at different temperature range. The new data may provide a further chance to improve the theoretical model developed recently for the interpretation of the behaviour of elastic constants in higher temperature region.

II. Formulation

Using Taylor's series expansion the elastic energy density[14] for a divalent crystal of a cubic symmetry can be expanded up to quartic terms as

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

Where α_{ij} are the Lagrangian Strain components, C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$ are the SOECs, TOECs and FOECs[15] in tensorial form. The SOECs, TOECs and FOECs are as given below:

$$C_{ijkl} = C_{IJ} = (\partial^2 U/\partial\alpha_{ij}\,\partial\alpha_{kl})_{\alpha=0}$$
$$C_{ijklmn} = C_{IJK} = (\partial^3 U/\partial\alpha_{ij}\,\partial\alpha_{kl}\,\partial\alpha_{mn})_{\alpha=0}$$

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

Where C_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations[16,17].

The free charge density of a crystal at a finite temperature T is

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

Where $U^{vib} = KT/NV_c \sum_{i=1}^{3sN} ln\ 2\ Sinh\ (\hbar\omega_i/KT)$

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 can be separated into two parts as follows,

$C_{IJ} = C^0_{IJ} + C_{IJ}^{vib}$, $C_{IJK} = C^0_{IJK} + C_{IJK}^{vib}$ and $C_{IJKL} = C^0_{IJKL} + C_{IJKL}^{vib}$ (3)

Table 1

The second order elastic constants and third order elastic constants in 10^{10} Newton/m^2 at room temperature for Potassium Halides

Crystal	Melting Point, K	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	Ref
KF	1136.00	6.989	1.235	1.366	-117.99	-6.874	1.122	3.012	3.012	-6.859	
		6.564	1.878	1.236							18
KCl	1098.321	3.654	1.023	0.899	-80.881	-2.363	0.041	1.455	-3.524	1.145	
		3.747a	0.859a	0.744a	-71.2b	-2.1b	1.5b	2.4b	2.4b	1.5b	18a,19b
						-2.11	0.99	1.021	-2.203	1.45	20
KBr	1001.00	3.012	0.653	0.748	-70.992	-2.014	-0.088	1.548	-3.011	1.450	
		3.250	0.878	0.474							18
KI	998.00	2.412	0.878	0.547	-55.332	-1.145	-0.298	1.069	-2.143	1.018	
		2.144	0.458	0.401							18

Table 2

The fourth order elastic constants in 10^{10} Newton/m^2 at room temperature of Potassium 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
KF	181	2.56	3.25	-1.12	-0.878	-0.621	-0.698	0.254	0.747	-0.298	-1.12	
	1701	21	30.12	-7.11	-7.01			29.0		29.0		21
	1812	31.212	40.69	-6.22	-5.12			29.12	-4.55	31.29		22
KCl	121	0.914	0.696	-0.489	-0.587	-0.478	-0.388	-0.414	-0.369	-0.589	-0.610	
	1145	17	19.99	-2.45	-3.012			24.7		28.1		21
	1289	12.45	-0.06	-1.01	-0.89			14.02	2.77	16.23		22
KBr	109	0.542	0.625	-0.487	-0.369	-0.889	-0.323	-0.501	-0.299	-0.721	-0.532	
	899	19	21.7	-2.02	-2.93			28.21		29.74		21
	1088	13.02	-5.85	-0.45	-0.09			11.96	-1.05	17.01		22
KI	89.23	0.456	0.412	-0.369	-0.302	-0.896	-0.256	-0.611	-0.289	-0.745	-0.451	
	788	25	26.89	-1.74	-2.92			34.03		36.01		21
	963	12.22	-1.88	-0.14b	-0.21			11.99	-1.86	15.09		22

Table 3

The fourth order pressure derivatives and second order pressure derivatives in 10^{-11} Newton/m^2 of the second order elastic constants and partial contractions of Potassium 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
KF	1877	78.2	77	09.59	1.45	-0.03	4.22	4.88	-5.89	-1.01	-0.56	
									-5.45	-0.36	-0.86	22
									-5.58	-1.14	-0.797	23
KCl	-11.78	-25.41	-5.85	10.58	1.65	-0.29	4.99	5.25	-14.9	-1.11	-1.01	
				11.97a	1.65a	-0.31a			-8.027b	-0.69b	-1.09b	
									-13.69	-1.45	-1.17	25a,22b
												23
KBr	-3.045	-12.458	-2.488	12.45	1.63	-0.41	5.05	5.74	-11.5	-2.01	-1.65	
									-11.85	-0.26	-2.87	22
									-12.83	-1.47	-1.26	23
KI	-0.03	-6.92	-1.08	11.98	1.56	-0.27	5.09	5.17	-16.01	-2.23	-2.47	
									-15.02	-1.12	-4.03	22
									-11.79	-1.81	-1.40	24
									-16.25	-2.46	2.02	23

Table 4

The nearest neighbour distance (r_0) and hardness parameter (q)

Crystal	r_0	Q	dC_{111}/dP	dC_{112}/dP	dC_{123}/dp	dC_{144}/dP	dC_{166}/dP	dC_{456}/dp	Ref
KF	2.5857	0.214	10.23	199	194	-1.23	71.23	2.47	
			-145	-4.71	2.89	1.02	1.63	2.01	22
KCl	3.412	0.287	0.47	125	131	-1.28	45.65	2.56	
			-153	-5.17	1.23	0.09	0.58	2.81	22
KBr	3.4526	0.411	-54.25	80.69	86.20	-1.03	28.0	1.88	
			-154	-6.11	1.12	0.09	-0.69	2.13	22
KI	3.9685	0.250	-72.0	61.9	70.01	-1.86	23.89	1.98	
			-178	-10.8	1.12	0.01	-2.35	2.46	22

Table 5

Numerical Coefficient for Potassium Halides.

Coefficient	A_1	A_2	A_3	A_4	A_5
KCl	-1.6721	0.2965	-8.1002×10^{-4}	9.2603×10^{-7}	-3.6254×10^{-10}
KBr	-0.7125	0.4102	-1.2874×10^{-3}	1.8114×10^{-6}	-8.5511×10^{-10}
KI	4.3569	0.3401	-1.1102×10^{-3}	1.5461×10^{-6}	-7.4611×10^{-10}

III. Result and Discussion

The second, third and fourth order elastic constant for Potassium Halide crystals are evaluated at different temperatures using the concept of hardness parameter and nearest neighbour distance. The second order elastic constant in 10^{11} dyn/cm^2 or Potassium Halide crystal at room temperature are shown in Table no. 1 along with available experimental data. It is clear that all SOECs are positive in nature and these values are depended on the temperature. We see that the anomalous temperature dependent of C_{12} does not occur in Potassium Halides crystal.

The TOECs which are evaluated at the room temperature are shown in Table no. 2. There are six TOECS for Potassium Halides at room temperature. The value of C_{144} are positive in nature and value of C_{111} and C_{166} negative in the nature. The TOECs or Potassium Halides are in well agreement with the experimental result which conclude that the validity of the present work for Potassium Iodide that elastic constant are sensitive to temperature while other Potassium Halide are not.

There are eleven fourth order elastic constant (FOECs) which are evaluated at the room temperature for Potassium Halide crystals. The result is shown in Table no. 3. The second order pressure derivative and fourth order pressure derivative of SOECs for Potassium Halide crystals are evaluated and shown in Table no. 4 & 5.

The overall, the presented are in well arrangement with the experimental data. The evaluated data are helpful for those researchers which are actively working in the present area. The evaluated data are very helpful for explaining and understanding non-linear behaviour of Potassium Halide crystals.

IV. References

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