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Temperature and Pressure Derivatives of Higher Order Elastic Constants of RBI

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Abstract:
In the present work a theory has been developed for quantifying the second order elastic constants, third order elastic constants and fourth order elastic constants, first order pressure derivatives of second and third order elastic constants, second order pressure derivatives of second order elastic constants and partial contractions for Rubidium Iodide crystal(from 50K up to 650K, near melting point of RbI) also. The results are discussed and compared with both experimental and theoretical data available in literature. The systematic analysis of data of Rubidium Iodide Crystals obtained through different techniques gives important and valuable information about its internal structure, anharmonic and inherent properties.

Keywords: *Elastic constants, pressure derivatives, temperature derivatives and partial contractions*

1. Introduction

In the present decade, considerable interest has been taken in investigation of anharmonic properties of materials of various kinds. While expanding elastic energy density for a deformed crystal using Taylor's series expansion, one gets a series with higher order coefficients. These coefficients are known as higher order elastic constants. In this expansion, the second, third and fourth order elastic constants are the coefficients of second, third and fourth order terms. When the values of these elastic constants of substance are known, many of the anharmonic properties of the substances can be treated within the limit of the continuum approximation in a quantitative manner. Several physical properties and crystal anharmonicities such as thermal expansion, specific heat at higher temperature, temperature variation of acoustic velocity and attenuation, the first order pressure derivatives of second order elastic constants and Grüneisen numbers can be quantified after discussing higher order anharmonicities such as the first order pressure derivatives of third order elastic constants, the second order pressure derivatives of second order elastic constants, partial contractions and deformation of crystals under large forces. In present decade considerable interest has been taken in investigation of anharmonic properties of materials of various kinds [1-10]. No complete experimental or theoretical efforts have been made so for in obtaining the temperature variation of anharmonic properties of materials possessing different crystal structures. The present work is concerned with the formulation to evaluate the second, third and fourth order elastic constants at an elevated temperature, the first order pressure derivatives of second and third order elastic constants, the second order pressure derivatives of second order elastic constants, partial contractions and first order temperature derivatives of second order elastic constants using long - and short - potentials starting from the nearest neighbour distance and hardness parameter for Rubidium iodide crystals.

2. Formulation

The elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as shown below [11];

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

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

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

and

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

C_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs.

The elastic constants consist of two parts as follows:

$$C_{IJ} = C^0_{IJ} + C_{IJ}^{vib}, \quad C_{IJK} = C^0_{IJK} + C_{IJK}^{vib} \text{ and } \quad C_{IJKL} = C^0_{IJKL} + C_{IJKL}^{vib} \qquad (2)$$

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 0K.

3. Evaluation

The theory for the calculating different anharmonic properties related constants of the substances possessing FCC crystal structures has been represented in the preceding section 2. Using the concept of nearest-neighbour distance and hardness parameter; the second, third and fourth order elastic constants for Rubidium iodide (RbI) are evaluated at different temperature (50K to up to their melting points). The values of the second, third and fourth order elastic constants at 300K for Rubidium iodide crystals are given in Tables (1 - 3). The FOPDs of SOECs and TOECs, the SOPDs of SOECs and partial contractions for this material are evaluated utilizing room temperature data of Tables (1 - 3) and the results are shown in Table 4 and 5. Table 6 present the value of FOTDs of SOECs at room temperature.

4. Results and Discussions

The SOECs, TOECs and FOECs in 10^{11}dyne/cm^2 at room temperature for Rubidium iodide are shown in Tables (1 – 3). The FOPDs of the SOECs and TOECs of Rubidium Halides are presented in Table 4.The SOPDs of the SOECs in 10^{-10} cm^2/dyne are shown in Table 5 and Partial Contractions in 10^{13} dyne/cm^2 are shown in Table 5. The calculated data of FOTDs of the SOECs for Rubidium iodide (RbI) are present in Table 6. The comparative values [12] of all anharmonic constants have been shown in tables.

The temperature variation of various anharmonic constants such as temperature variation of SOECs, TOECs and FOECs, FOPDs of SOECs and TOECs, the SOPDs of SOECs, partial contractions and FOTDs of the SOECs are represented graphically for Rubidium iodide. It may be stated that all the SOECs are positive in nature. From figure (1) the value of $C_{11}$and C_{44} increases and the value of C_{12} decreases as temperature increases .Out of six third order elastic constants for Rubidium iodide at 300K, C_{111}, C_{112} and C_{166} are negative in nature while C_{123}, C_{144} and C_{456} are positive in nature. The experimental value [13] of SOECs and TOECs for RbCl are present in Table (1-2). Figure (2) shows the value of $C_{111}$and C_{112} increases, but C_{123} decreases as temperature increases. There are eleven fourth order elastic constants for Rubidium iodide. From figure (3) the value of C_{1111}, C_{1112} and C_{1122} decreases as temperature increases. Figure (4) present the temperature variation of first order pressure derivatives of second order elastic constants for Rubidium iodide. The value of dC_{11}/dp and dC_{12}/dp decreases and the value of dC_{44}/dp somewhere increases or decreases as temperature increases. Figure (5) presents the values of d^2C_{11}/dp, d^2C_{12}/dp and d^2C_{44}/dp which decrease as temperature increases for Rubidium iodide. From Figure (6) one can say that the value of dC_{11}/dT, dC_{12}/dT and dC_{44}/dT decreases as temperature increases for Rubidium iodide. The experimental and theoretical data [14-18] obtained by other authors have been shown in tables which is available in literature. The cases discussed in the present study are overall in good agreement with theoretical and experimental results, which shows the validity of the present theory. The data obtained in present investigation will be helpful to those workers [19-22] who are engaged in such studies.

5. References

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Annexure

Comp.	Mel. Point	r_0	q	C_{11}	C_{12}	C_{44}	Reference
RbI	647^0c	3.6220	0.415	2.609 3.188 3.210	0.494 0.324 0.361	0.568 0.512 0.292	Present [12] Exp.[13]

Table 1: The Nearest-neighbour distance (r_0) and hardness parameter (q) in 10^{-8}cm and SOECs in 10^{11} Dyne/cm^2 at room temperature for Rubidium Iodide

Comp.	q	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	References
RbI	0.315	-46.346 -54.64 -50.72	-13.955 -1.125 -1.223	0.918 0.455 0.002	1.031 0.929 0.882	-1.915 -2.004 -1.744	0.909 0.909 0.856	Present [12] Exp.[13]

Table 2: TOECs in 10^{11} Dyne/cm^2 at Room Temperature for Rubidium Iodide

Comp	C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1155}	C_{1255}	C_{1266}	C_{1456}	C_{4444}	C_{4455}	Ref.
RbI	-302.3 692.4 1197.7	-180.8 -37.36 10.45	-106.2 -47.60 -46.95	-0.868 -50.09 -0.840	-2.269 -2.217 -0.242	6.148 7.126 8.995	-3.276 -2.157 -2.156	9.201 11.34 8.693	-2.124 2.125 -1.857	10.56 11.55 12.22	-2.138 -2.127 0.634	 [12] [14]

Table 3: FOECs in 10^{11} Dyne/cm^2 at room temperature for Rubidium Iodide

Comp.	$\frac{dC_{11}}{dP}$	$\frac{dC_{12}}{dP}$	$\frac{dC_{44}}{dP}$	$\frac{dC_{111}}{dP}$	$\frac{dC_{112}}{dP}$	$\frac{dC_{123}}{dP}$	$\frac{dC_{144}}{dP}$	$\frac{dC_{166}}{dP}$	$\frac{dC_{456}}{dp}$	Reference
RbI	-20.450 -13.00 13.66	-9.487 1.45 1.38	-0.297 -0.33 -0.34	249.87 -115	100.38 35.1	0.954 40.5	1.160 -1.14	2.890 14.9	2.121 1.95	Present [12] [15]

Table 4: The First Order Pressure Derivatives of the Second and Third Order Elastic Constants for Rubidium Iodide

Comp.	$\frac{d^2C_{11}}{dP^2}$	$\frac{d^2C_{12}}{dP^2}$	$\frac{d^2C_{44}}{dP^2}$	Y_{11}	Y_{12}	Y_{44}	Reference
RbI	10.244 18.26 -18.4	3.539 -1.65 -2.3	5.285 0.24 -1.3	-12.397 3.476 7.7	-5.784 -4.204 -0.41	0.140 -0.747 0.21	Present [12] [16]

Table 5: The SOPDs of the SOECs in 10^{-10} (Dyne/cm^2)$^{-1}$ and Partial Contraction (Y□ in 10^{13}Dyne/cm^2 for Rubidium Iodide

Comp.	$\frac{dC_{11}}{dT}$	$\frac{dC_{12}}{dT}$	$\frac{dC_{44}}{dT}$	$\frac{dC_{13}}{dP}$	$\frac{dC_{15}}{dP}$	$\frac{dC_{17}}{dP}$	Reference
RbI	-2.715 -1.798 -2.251	-0.948 0.099 0.001	-0.248 -0.109 -0.052	-2.588 -1.676	-1.047 -0.023	-0.121 0.001	Present [17] [18]

Table 6: The First Order Temperature Derivatives of the Second Order Elastic Constants for Rubidium Iodide

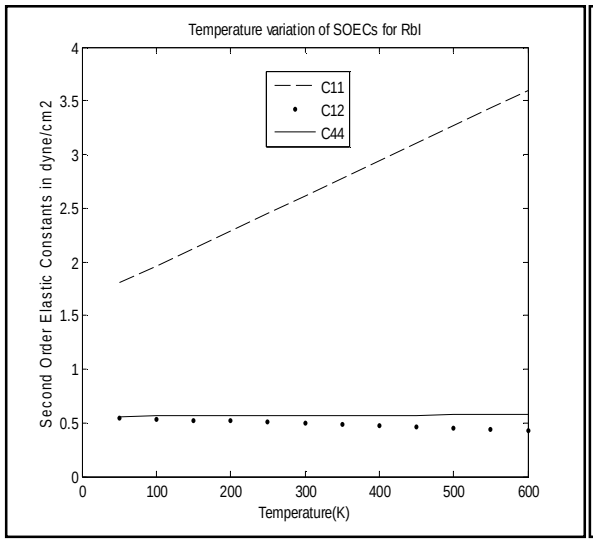

Figure 1

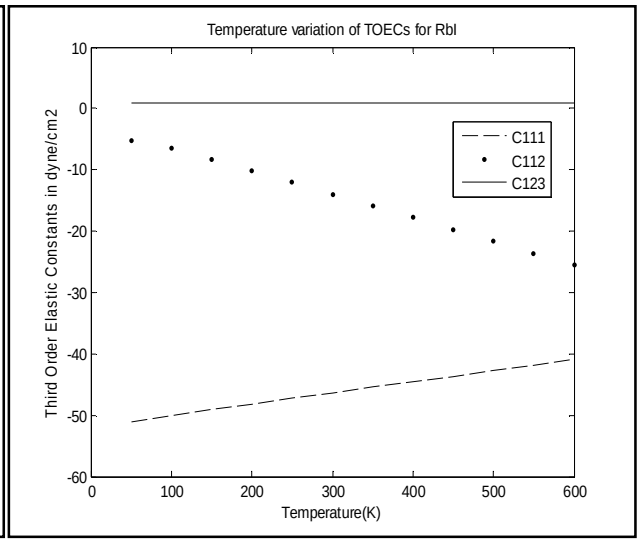

Figure 2

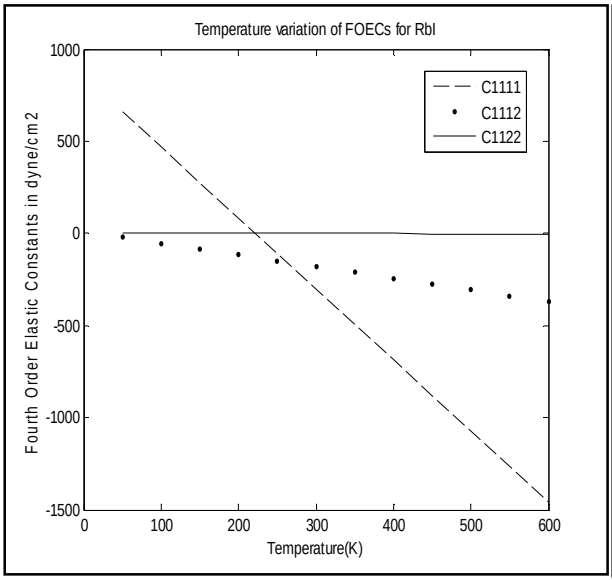

Figure 3

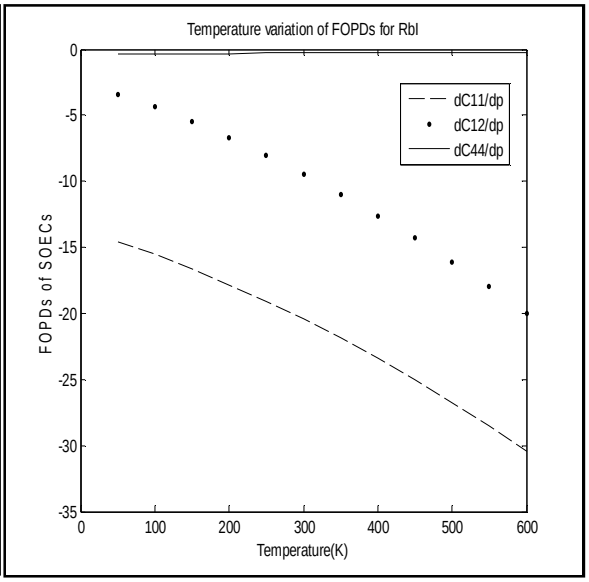

Figure 4

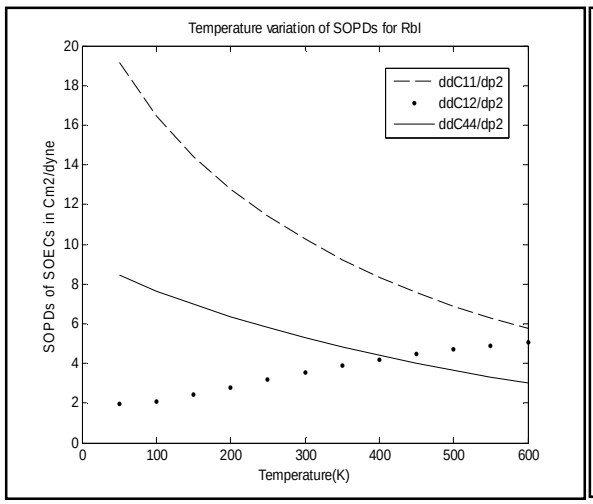

Figure 5

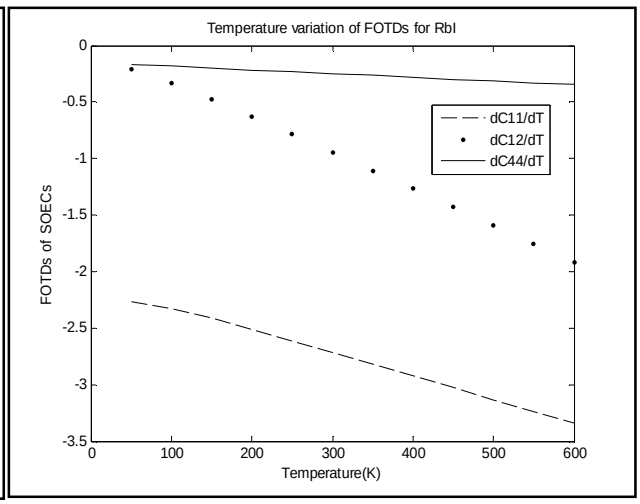

Figure 6