

Lattice Theory of Fourth Order Elastic Constants of Primitive Lattices

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ABSTRACT	The lattice theory of fourth order elastic constants for primitive lattices derived by S.C. Goyal and K. Kumar [3] is applied to obtain the relations for the FOE constants of NaCl structure types solids within the framework of the Lundqvist many body potential the derived relations of FOEC are used to compute the numerical values of the FOE Constants and second order pressure derivatives of the SOE Constants of Rubidium halide solids.
KEYWORDS	Elastic Constant, Lattice theory, Elasticity.

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INTRODUCTION

The study of the higher order elastic constants of solids plays an important role in analyzing the various anharmonic properties of the solids. In this direction Garg et al. [1] and Mori and Hiki [2] have formulated theoretical expressions using the homogeneous deformation theory to study the Fourth Order Elastic (FOE) constants of cubic structure solids.

S.C. Goyal and K. Kumar [3] have also reported a theoretical approach using a macroscopic theory of elasticity [4] and the lattice theory [5] of elasticity to study the FOE constants of the cubic structure solids. The present paper deals with the application of a lattice theory [6] to obtain the analytical expression of the FOE constants NaCl type cubic structure solids. The derived relations of FOE constants are also used to evaluate the values of second-order pressure derivative of the SOE constants of Rubidium halides.

THEORY

The expressions of the FOE constants for the primitive lattice relations (25a-k) derived by authors (3) for NaCl type structure solids are as follows:–

$$\begin{aligned}
 C_{1111} &= \frac{e^2}{4a^4} \left[-305.3585\epsilon(\epsilon + 12f(r)) + D_1 - 6C_1 + 15A_1 + 18.6411\epsilon \left(a^3 \frac{d^3 f}{dr^3} \right) \right. \\
 &\quad \left. - 206.5708\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) + 863.4907\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1112} &= \frac{e^2}{4a^4} \left[17.9035\epsilon(\epsilon + 12f(r)) + 4.6602\epsilon \left(a^3 \frac{d^3 f}{dr^3} \right) + 2.7111\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) \right. \\
 &\quad \left. + 103.4886\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1122} &= \frac{e^2}{4a^4} \left[22.4611\epsilon(\epsilon + 12f(r)) - 50.2157\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) - 27.1578\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1123} &= \frac{e^2}{4a^4} \left[-6.3409\epsilon(\epsilon + 12f(r)) + 5.5640\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) - 22.5135\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1144} &= \frac{e^2}{4a^4} \left[-6.3409\epsilon(\epsilon + 12f(r)) + 5.5640\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) + 16.1732\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1166} &= \frac{e^2}{4a^4} \left[27.2240\epsilon(\epsilon + 12f(r)) + 8B_1 + 5.5640\epsilon \left(a^2 \frac{d^2 f}{dr^2} \right) - 44.2508\epsilon \left(a \frac{df}{dr} \right) \right] \\
 C_{1244} &= \frac{e^2}{4a^4} \left[-6.3409\epsilon(\epsilon + 12f(r)) - 8.4747\epsilon \left(a \frac{df}{dr} \right) \right]
 \end{aligned}$$

$$\begin{aligned}
C_{1266} &= \frac{e^2}{4a^4} [27.1214\epsilon(\epsilon + 12f(r)) + 4B_1 - 38.6868\epsilon \left(a \frac{df}{dr}\right)] \\
C_{1456} &= \frac{e^2}{4a^4} [-6.3409\epsilon(\epsilon + 12f(r)) + 10.8686\epsilon \left(a \frac{df}{dr}\right)] \\
C_{4444} &= \frac{e^2}{4a^4} [32.9468\epsilon(\epsilon + 12f(r)) + 9B_1] \\
C_{4466} &= \frac{e^2}{4a^4} [-4.0108\epsilon(\epsilon + 12f(r)) + 2B_1]
\end{aligned} \tag{1a-k}$$

NUMERICAL CALCULATIONS AND DISCUSSION

The calculated value of model parameters A_1 , B_1 , C_1 , D_1 , $f(r)$, $\left(a \frac{df}{dr}\right)$, $\left(a^2 \frac{d^2f}{dr^2}\right)$ and $\left(a^3 \frac{d^3f}{dr^3}\right)$ are listed in Table-1.

Table 1: Calculated value of model parameters

Compound	A_1	B_1	C_1	D_1	$f(r)$	$\left(a \frac{df}{dr}\right)$	$\left(a^2 \frac{d^2f}{dr^2}\right)$	$\left(a^3 \frac{d^3f}{dr^3}\right)$
RbCl	10.1619	-0.7894	-30.8135	1683.9551	-0.0269	0.0313	0.1389	-2.4743
RbBr	10.3979	-0.7747	-139.5590	1873.1381	-0.0279	0.0290	0.6298	-18.4741
RbI	10.5015	-0.7308	-150.9052	2168.4875	-0.0311	0.0296	1.0031	-25.3895

Substitute the values of above model parameters relations (1a-k). The results are given in Tables 2

Table 2: Calculated values of FOE constants (in 10^{11} dyn/cm²)

	RbCl	RbBr	RbI
C_{1111}	1167.426	909.496	759.845
C_{1112}	2.080	-28.542	-32.276
C_{1122}	3.648	-7.180	-11.815
C_{1123}	-2.086	-0.561	0.299
C_{1144}	-1.489	-0.100	0.663
C_{1166}	5.683	5.834	4.939
C_{1244}	-2.250	-1.833	-1.347
C_{1266}	6.911	5.675	4.124
C_{1456}	-1.952	-1.603	-1.165
C_{4444}	7.508	6.136	4.489
C_{4466}	-2.120	-1.732	-1.267

Table 3: Second pressure derivatives of SOE constants (in 10^{-11} cm²/dyn)

Crystal	$\frac{d^2c_{11}}{dp^2}$		$\frac{d^2c_{12}}{dp^2}$		$\frac{d^2c_{44}}{dp^2}$	
	Calculated	Exp.(6)	Calculated	Exp.(6)	Calculated	Exp.(6)
RbCl	-11.3	-11.3 ± 1.7	-0.28	-0.30 ± 2.6	-0.97	-1.1 ± 0.4
RbBr	-15.6	-15.6 ± 2.7	-3.92	-3.5 ± 3.6	-0.64	-1.2 ± 0.2
RbI	-18.6	-18.6 ± 2.6	-5.71	-2.3 ± 4.0	-0.45	-1.3 ± 0.4

It is clear from table 2 that the values of FOE constants for all the three RbCl, RbBr, RbI halides are much larger in magnitude as compared to the values of TOE or SOE constants. These halides showing that the expansion of potential function is converging slowly and the higher order anisotropy is present there more over the calculated values of longitudinal constants C_{1111} in case of all three halides are larger than the calculated values of the other ten transverse constants.

Due to the lack of experimental data on the FOE constants in case of these halides, we have checked the derived relations by calculating the second pressure derivatives of the SOE constants as the experimental data of these constants for the crystals under study are available.

CONCLUSION

It is interesting to note from Table 3 that the calculated values of $\frac{d^2c_{ij}}{dp^2}$ are in good agreement with the corresponding experimental values. Thus the present theory is more general than the earlier reported study of pressure derivatives of SOE constants [7,8,9], Therefore, it may be useful in the further study of elastic behavior of cubic structure solids.

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