Calculation of Three Body Potentials In Rubidium Halides

M REKHA RANI[#1], B SRINIVASA RAO[*2]

[#] Department of Physics, SICET(Autonomous), Hyderabad-501510,India.
[*]Department of Physics, GRIET(Autonomous), Hyderabad-500090, India.
[1]maddularekharani@gmail.com
[2]bmsssaditya_1997@yahoo.co.in

Abstract: In the current work we have got studied the pressure-induced structural phase change and elastic constants at high pressure for two Rubidium halide crystals specifically RbCl and RbBr. The study is formed using a model potential that has many-body interactions because of electron shell overlap.

Keywords: Computer simulation, phase transition, Many- body interactions, and Elastic constants.

I. INTRODUCTION

The alkali halides are standard to endure a structural phase transformation from B1 (NaCl) to B2 (CsCl) structures between 0 .5 Gpa to 30 Gpa [1]. No nonconductor to metal transition in these solids has been reportable so far. many theoretical makes an attempt have been made by varied employees to interpret the equation of states, phase change pressures victimization each ab intio and model theories [2-5]. With the availabilities of additional precise experimental information [6], it's been found that these theories are quite inadequate to elucidate the equation of states of easy ionic solids. Model calculations victimization Born – Mayer sort potential [5] and therefore the the respiration shell models have also been not prospering in finding an honest agreement with the experimental results, because the correction owing to electron shell deformation at high pressure has not been thought-about in their potential functions. within the gift work, we have a tendency to investigate the results of the many-body interactions on structural section transitions and elastic constants of rubidium Halides.

II. MODEL POTENTIAL

The details of the three- body interaction (TBI) potential are identical as reported by Jog et al [7]. Here we tend to use shortly outline some of the helpful features of the TBI potential. The potential energy of the alkali halides is expressed as which incorporates long-range coulomb (first term), 3 –body interaction (second term), Vander Walls multiple interactions (third term) and Hafemeister and Flygare variety of short-range repulsive energies (last term). This potential has 5 parameters b, ρ, f(r). The TBI parameter f(r) has the useful type $f(r) = fo.\exp(- rij / \rho_{ij})$ and is considered to be effective up to the primary nearest neighbors solely [7]. the upper order derivatives f(r) are often evaluated by assumptive the higher than useful type. Moreover, their parameter has been thought of structure dependent. The short ranges parameters ij and f(r) are obtained from overlap integrals [8]. the only parameter b has been fitted to equilibrium inter ionic separation.

$$U(r) = \frac{1}{2}\sum_{kk'}^{1}\frac{z_k z_{k'} e^2}{|\vec{r}_{kk'}|} + \frac{1}{2}\sum_{kk'k''}^{1}\frac{z_k z_{k'} e^2}{|\vec{r}_{kk'}|} f(r_{kk''}) + \sum_{kk'} c_{kk''} r_{kk''}^{-6} + \sum_{kk'} D_{kk''} r_{kk''}^{-8} + \sum_{kk'} b\beta_{kk'} \exp[r_k + r_{k'} - r_{kk'} / \delta_{kk'}) \quad (1)$$

III.METHOD OF CALCULATION

The phase transition pressure (p_t) at that ΔG (=G_{B1} –G_{B2}) becomes zero may be calculated from the model at T = 0K victimization the tactic mentioned by jog et al [7]. Gibbs free energy GB1 corresponds to NaCl (B1) part may be expressed as $G_{B1}(r) = U^{B1}(r) + 2\ pr^3$ wherever UB1 is given by eq (1). The Gibbs free energy similar to CsCl structure may be written with necessary modification. the primary order natural action involving a separation in volume takes place at transition pressure.

IV.RESULTS AND DISCUSSION

In the present work, the structural phase transition pressure and elastic constants are computed for 2 rubidium salt crystals RbCl and RbBr and compared with experimental information [9-14]. The phase diagrams for RbCl and RbBr are shown in fig.1 and 2 severally. The cohesive and phase change properties of rubidium halides are bestowed in Table-I. Table-II consists of the whole values of elastic constants of sodium halides of zero pressure and and also the sher instability.

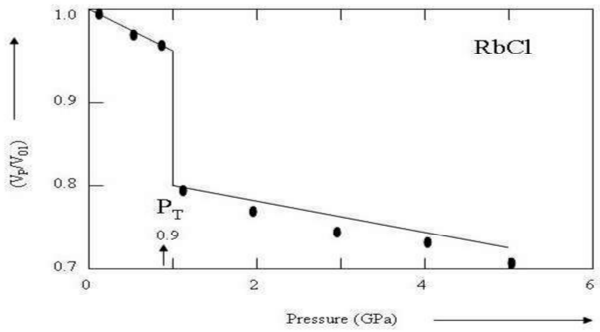

Fig. 1. Phase Diagram Of Rbcl

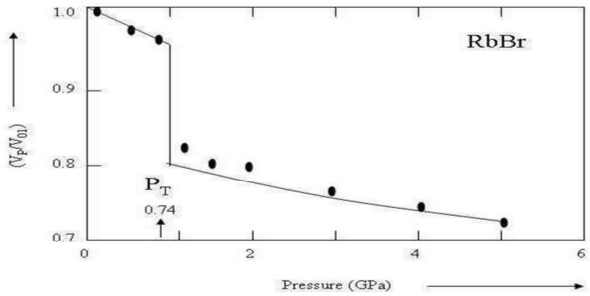

Fig. 2. Phase Diagram Of Rbbr

From Fig 1 and 2, it isdetermined that the phase diagrams of RbCl and RbBr, this inter-ionic potential has satisfactorily explained the cohesive and phase transition properties of the rubidium halides. The equilibrium lattice constant and cohesive energy of those crystals are in superb agreement with the experimental results. The computed phase transition pressures for the RbCl and RbBr are in fairly in agreement with the experimental values when put next with the opposite theoretical computations. Also, the relative volume amendment

(-ΔV / Vo1) is inconsistent with the offered experimental values. The experimental price of phase transition pressure (p_t) according are at temperature, whereas the calculated values area unit 0K. so the temperature impact will simply explain the deviation of this theoretical value from the experiment. The calculated values of zero pressure elastic constants for the RbCl and RbBr and are conferred in Table-II and compared with the experimental and different theoretical values. we have a tendency to observe a fairly good agreement from our present model that does not use these constants for the determination of those parameters. Also, we've according the Cauchy violation a lot of or less satisfactorily. lastly, we've studied the natural action pressures and elastic constants of 2 rubidium halide crystals RbCl and RbBr severally using a semi-empirical many-body potential model that predicts a lot of or less accurately the transition pressure and elastic constants.

Table I.
Cohesive And Phase Transition Properties Of Rubidium Halides

Crystal	Models	Equilibrium lattice constant		Cohesive Energy (KJ/mole)		Phase Transition Pressure (GPa) at room temp	Relative Volume change % $(-\Delta V/V_0)$
		$R_1(B_1)$ (Å)	$R_2(B_2)$ (Å)	$U_1(B_1)$	$U_2(B_2)$		
1. RbCl	Present	3.26	3.34	-700.98	-694.80	0.90	16
	Expt	3.29[a]	--	-683.98[b]	--	0.55[e]	14[e]
	Theory	--	--	-515.16[c]	--	1.71[e]	--
	Theory	--	--	-485.26[d]	--	2.90[f]	--
2. RbBr	Present	3.49	3.57	-658.09	-651.81	0.78	16
	Expt	3.44	--	-656.98[b]	--	0.50[e]	13[e]
	Theory	--	--	-485.26[c]	--	9.70[e]	--
	Theory	--	--	-643.47[d]	--	2.40[f]	--

Table II.
Elastic Properties Of Rubidium Halides

Crystal	Model	C_{11} (Gpa)	C_{12} (Gpa)	C_{44} (Gpa)	B (Gpa)
RbCl	Present	44.21	7.40	7.70	19.67
	Expt[a]	44.99	6.70	4.92	19.46
RbBr	Present	33.54	5.76	6.27	15.52
	xpt	33.63	4.70	4.09	16.01

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