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Computer Simulation Study of Structural Phase Transition and Elastic Properties of Rubidium Halides

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Abstract: In the present work, we have studied the pressure-induced structural phase transition and elastic constants at high pressure for two Rubidium Halide crystals namely RbCl and RbBr. The study is made using a model potential that includes many body interactions due to electron shell overlap.

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

1. INTRODUCTION

The alkali halides are well known to undergo a structural phase transformation from B1 (NaCl) to B2 (CsCl) structures between 0 .5 Gpa to 30 Gpa [1]. No insulator to metal transition in these solids has been reported so far. Several theoretical attempts have been made by various workers to interpret the equation of states, phase transition pressures using both ab intio and model theories [2-5]. With the availabilities of more precise experimental data [6] it has been found that these theories are quite inadequate to explain the equation of states of simple ionic solids. Model calculations using Born – Mayer type potential [5] and the breathing shell models have also been not successful in finding a good agreement with the experimental results, as the correction due to electron shell deformation at high pressure has not been considered in their potential functions. In the present work, we investigate the effects of the many-body interactions on structural phase transitions and elastic constants of Rubidium Halides.

2. MODEL POTENTIAL

The details of the three- body interaction (TBI) potential are the same as reported by Jog et al [7]. Here we use briefly outline some of the useful features of the TBI potential. The potential energy of the alkali halides is expressed as which includes long-range coulomb (first term), three –body interaction (second term), Vander Walls multiple interaction (third term) and Hafemeister and Flygare form of short – range repulsive energies (last term). This potential has five parameters b, ρ, f(r). The TBI parameter f(r) has the functional form $f(r) = f_o.\exp(-r_{ij} / \rho_{ij})$ and is considered to be effective up to the first nearest neighbors only [7]. The higher order derivatives f(r) can be evaluated by assuming the above functional form. Moreover their parameter has been considered structure dependent. The short ranges parameters ρ_{ij} and f(r) have been obtained from overlap integrals [8]. The only parameter b has been fitted to equilibrium inter ionic separation.

$$U(r) = \frac{1}{2}\sum_{kk^1}^{1}\frac{z_k z_{k^1} e^2}{\left|\vec{r}_{kk^1}\right|} + \frac{1}{2}\sum_{kk^1 k^{11}}^{1}\frac{z_k z_{k^1} e^2}{\left|\vec{r}_{kk^1}\right|} f(r_{kk^{11}}) + \sum_{kk^1} c_{kk^{11}} r_{kk^{11}}^{-6} + \sum_{kk^1} D_{kk^{11}} r_{kk^{11}}^{-8} + \sum_{kk^1} b\beta_{kk^1} \exp[r_k + r_{k^1} - r_{kk^1} / \delta_{kk^1}) \quad (1)$$

3. METHOD OF CALCULATION:

The phase transition pressure (p_t) at which ΔG ($=G_{B1} - G_{B2}$) becomes zero can be calculated from the model at T = 0K using the method discussed by jog et al [7]. Gibbs free energy G_{B1} corresponds to NaCl (B1) phase can be expressed as $G_{B1}(r) = U_{B1}(r) + 2\,pr^3$ where U_{B1} is given by Eq (1). The Gibbs free energy corresponding to CsCl structure can be written with necessary modification. The first order phase transition involving a discontinuity in volume takes place at transition pressure.

4. RESULTS AND DISCUSSION

In the present work, the structural phase transition pressure and elastic constants have been computed for two Rubidium halide crystals RbCl and RbBr and compared with experimental data [9-14]. The phase diagrams for RbCl and RbBr are shown in fig.1 and 2 respectively. The cohesive and phase transition properties of Rubidium halides are presented in Table-I. Table-II consists of the complete values of elastic constants of sodium halides of zero pressure and the shear instability.

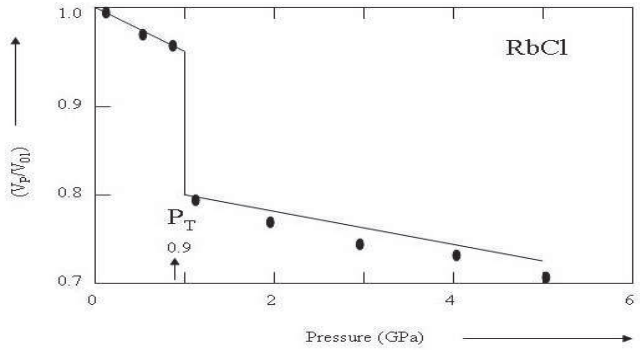

Fig. 1. Phase diagram of RbCl

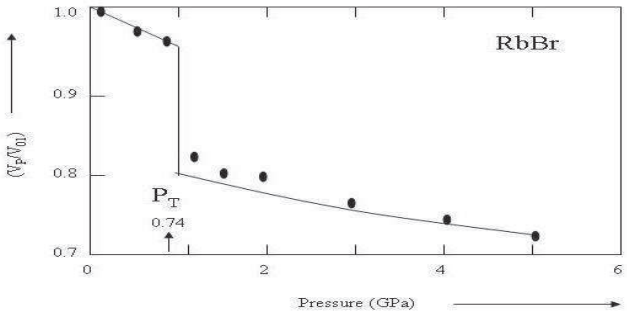

Fig. 2. Phase Diagram of RbBr

From Fig 1 and 2 it is observed that the phase diagrams of RbCl and RbBr, the present inter-ionic potential has satisfactorily explained the cohesive and phase transition properties of the Rubidium halides. The equilibrium lattice constant and cohesive energy of these crystals are in very good agreement with the experimental results. The computed phase transition pressures for the RbCl and RbBr are in reasonably in agreement with the experimental values when compared with the other theoretical computations. Also, the relative volume change (- ΔV / Vo1) is in consistent with the available experimental values. The experimental value of phase transition pressure (p_t) reported are at room temperature, while the calculated values are 0K. Thus the temperature effect can easily explain the deviation of the present theoretical value from the experiment. The calculated values of zero pressure elastic constants for the RbCl and RbBr and are presented in Table-II and compared with the experimental and other theoretical values. We observe a reasonably good agreement from our present model which does not use these constants for the determination of these parameters. Also we have reported the Cauchy violation more or less satisfactorily. In conclusion, we have studied the phase transition pressures and elastic constants of two Rubidium halide crystals RbCl and RbBr respectively using a semi – empirical many body potential model which predicts more 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
	Expt[a]	33.63	4.70	4.09	16.01

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