

STRUCTURAL ANALYSIS OF NAH UNDER HIGH PRESSURE AT ROOM TEMPERATURE

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ABSTRACT:

We have studied the pressure induced structural phase transformation in NaH compound by using realistic interaction potential (RIP) approach which considers Coulomb interaction; three body interaction and short range overlap repulsive interactions up to first neighbor including temperature effects. Our calculated results are in good agreement with experimental and better than other theoretical data.

KEYWORDS: *Phase transition, alkali metal, three body interaction*

1. INTRODUCTION

The alkali metal compounds AX (A=Na, K, Li and X= Cl, Br, H and I) are studied widely because of the simple structure and electronic configuration. These properties have stimulated many researchers to use first principle calculations. The phase change in solids at high pressure usually involves a change in crystal structure. On applying pressure the coordination number of solids gets changed. This is because thermodynamically the molar volume of low pressure phase must be higher than high pressure phase. Basshkin et al. [1] reported the B₁ to B₂ transition in alkali hydride compounds by using a hard-sphere ion model. Jain et al. [2] studied the structural phase transition of NaH from NaCl to CsCl by using the effective interionic potential model. Ahuja et. al. [3] predicted phase the transition pressure (P_t) at 37 GPa for NaH. Martins [4] have investigated P_t at about 39 GPa and 6.2 GPa respectively for NaH and KH by using the pseudopotential and local density approximation. Duclos et al. [5] investigated the P_t of NaH in the range 28-32 GPa experimentally. Rodriguez et. al [6] studied the structural properties of alkali halides by using an improved linear- Muffin-tin- orbital (LMTO)-atomic-sphere-approximation (ASA). As less work is reported for NaH by including the temperature effects, so we have devoted a realistic interaction potential approach to study the structural properties present compound. We have calculated the transition pressure and relative volume collapses under high pressure at room temperature. Our results are well fitted with experimental and other theoretical data.

2. METHOD OF CALCULATION

It is known that pressure causes a compression in the volume of crystals which leads to the transfer of charge and deformation of the overlapping electron shell. These transferred charges interact with all other charges in the overlap region of the lattice via. Coulomb's law and give rise to many body interaction (MBI) [7]. The dominant part of MBI is the three body interaction (TBI). To obtain the stability for a crystal structure, the effect of TBI has lattice energy, S is the vibrational energy at absolute temperature T , pressure P and volume V . The Gibbs free energy for rock salt (B_1 , real) and CsCl (B_2 , hypothetical) structure at $0K$ can be stated by:

$$G_{B_1}(r) = U_{B_1}(r) + PV_{B_1} - TS_1 \quad (1)$$

$$G_{B_2}(r') = U_{B_2}(r') + PV_{B_2} - TS_2 \quad (2)$$

With V_{B_1} ($=2.00r^3$) and V_{B_2} ($=1.54r'^3$) as the unit cell volumes, S_1 and S_2 are the entropies for B_1 and B_2 phases, respectively. For calculating the value of lattice energies, we have to determine the value of three model parameters (b , ρ , $f(r)$) namely hardness, range and three body force parameter. Their values have been find out by solving the equilibrium conditions ($\frac{dU}{dr} = 0$ and $\frac{d^2U}{dr^2} = 9k_{B_1}r$) using the measured values of the equilibrium inter-ionic separation (r). To obtain better compatibility with experimental results we have taken account of the room temperature in pressure induced theoretical calculations.

Now, the entropy differences in the last term of Eq. (1) and (2) can be calculated from the relation expressed in our previous work [8].

3. RESULTS AND DISCUSSION

Using the measured values of the equilibrium lattice constant (r) and bulk modulus (B_T) with $K=2$ for B_1 phase, the model parameters thus calculated are listed in Table 1 and are used to compute the results presented and discussed below. For simplicity, we have taken account of only a single set [ρ , b , $f(r)$] in B_1 -phase and the same set is used in B_2 phase. The reason for this is that during the phase transition from $B_1 \rightarrow B_2$ the atomic distribution takes a different arrangement and they get arranged in B_2 structure after phase transition and it also affects inter-ionic separation. Inter-ionic separation changes are calculated by the minimization technique. The parameter $f(r)$ is inter-ionic separation (r) dependent and it is therefore changed accordingly. The condition of relative stability of the two phases may be expressed as $\Delta G = (G_{B_2}(r') - G_{B_1}(r))$, where $G_{B_1}(r)$ and $G_{B_2}(r')$ are the Gibbs free energies for rock salt (B_1 , real) and CsCl (B_2 , hypothetical) structure. The pressure at which $\Delta G \rightarrow 0$ is the phase transition pressure P_t which is associated with a sudden collapse in volume. This shows that the phase transition is of first order. . At

this pressure both the phases coexist. ΔG is important factor in deciding the relative stability of phases. After phase transition system becomes stable in B_2 phase, the calculated value of phase transition and the associated relative volume change V_p/V_o is given in Table 2. The variations of ΔG against pressure at $T=0K$ and $T=300K$ are depicted in Fig.1. The variations of V_p/V_o against pressure at $T=0K$ and $T=300K$ are depicted in Fig.2.

TABLE 1. Input Parameters and Model Parameters

Solid	Input parameters		Model parameters		
	r(Å)	B_T (GPa)	b (10^{-12} erg)	ρ (Å)	f(r)
NaH	2.440 ^a	19 ^b	0.1272	0.3712	-0.0058

a. ref [9], b. ref [6]

TABLE 2. Calculated Transition Pressures and Volume Collapses

Solid	T (K)	Transition pressure (GPa)			Volume collapses (%)		
		present	exp	other	present	exp	other
NaH	0	30	-	30.7 ^a , 37 ^b , 37 ^c	9.70	-	8.8 ^a , 4.3 ^c
	300	28.50	28-32 ^d	-	10.15	10	

a. ref [6], b. ref [3], c. ref [2], d. ref [5]

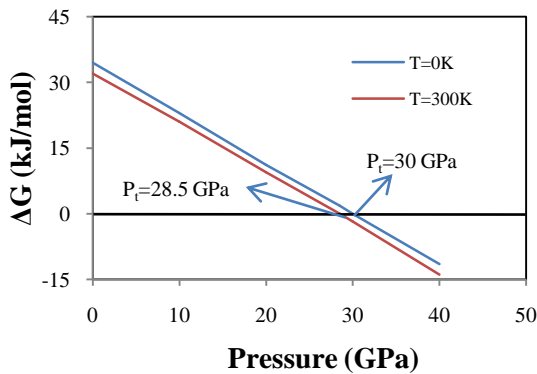


Fig.1 Variations of ΔG with Pressure for NaH

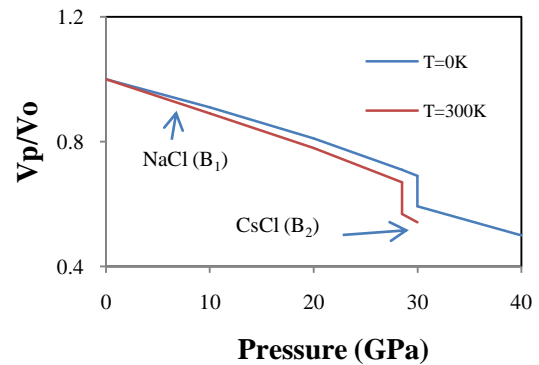


Fig.2 Variations of V_p/V_o with Pressure for NaH

Lastly, we can conclude that our (RIP) approach is found to be suitable for investigating the structural properties of NaH. The results obtained are well fitted with experimental data and better than other reported theoretical data.

4. CONCLUSION

In the present paper we investigated the phase transition pressure in NaH compound by using realistic interaction potential (RIP) approach. The result can be concluded as:

1. The lattice parameters have been varied to find the stability of the structures that corresponds to minimum total energy, NaH is stable in both the phases (B1 and B2).
2. Present approach is suitable for the calculation of B1 to B2 phase transition of NaH. It is to be noted that the results of the phase transition pressure is found to be in good agreement with the available data.

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