



## TITLE STUDY OF STRUCTURAL PROPERTIES OF ROCKSALT (B1)

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**Abstract-**In rock salt or sodium chloride structure each of the two different atom forms a separate face centered cubic lattice, with the two lattices interpenetrating so as to form a 3D checkerboard pattern. Generally, this structure is more likely to be formed if the cation is slightly smaller than the anion. The space group of this structure is Fm3m (225) and strukturbericht designation is. In this structure the coordination number of each atom is 6: each cation is coordinated to 6 anions at the vertices of an octahedron, and similarly, each anion is coordinated to 6 cations at the vertices of an octahedron. The rock salt structure has ccp/fcc anions with octahedral sites fully occupied by cations and tetrahedral sites empty. Each cation is surrounded by six anions and similarly, each anion is octahedrally coordinated by cations (to see this, consider the anion at the body centre. These materials are important promising engineering materials that are used in various industrial applications such as electronics, petroleum, aerospace, high power, high temperature engineering, nuclear industry and chemical industry [1-5]. These materials are partially covalent after certain range. Therefore, a number of experimental and theoretical workers have devoted their efforts to study the nature of these interactions, which are considered as a function of nearest and next nearest neighbours distance. Interacting forces in a crystal dictate the properties of the solid-state materials. To describe this effect the term mixed crystal is used. If the impurity ion behaves in the same charge to the Lattice ions. Wasastijerma [21] carried out a thorough study on mixed alkali halides and found that the mixed alkali halides reflected the X-rays as if they are homogeneous solutions. It should be realized that the impurity ions are all distributed randomly throughout the Lattice so that the term solid solution is more appropriate. In present study three body potential (TBP) has successfully explained both static and dynamical properties of materials with three different cubic structure, namely rock salt (RS). The chief aim of the present study is to reformulate the TBP by including the effects of the long range coulomb and three-body interaction as well as the van der Waals attraction ( $V_{dw}$ ) and overlap repulsion. We have applied this TBP model to the several mixed ionic solids.

### 1. INTRODUCTION

The choice of the primitive vectors of the Bravais face centered cubic lattice is similar as for zinc-blende but the position vectors of the two atoms, ( $i = 1, 2$ ), inside the unit cell, are given by

$$\mathbf{r}_1 = (0, 0, 0), \mathbf{r}_2 = (0.5a, 0.5a, 0.5a),$$

Where  $\mathbf{r}_1$  denote the vector position of the group III atoms (Ga or Al), while  $\mathbf{r}_2$  the X (=P, As, Sb) atoms.

According to classical theories of Born [6] the atoms are considered as point charges bond by the interaction forces which have attracted considerably the attention of theoretical and experimental workers due to their interesting and useful applications. The developments of such Lattice dynamical models have progressed from simple phenomenological to sophisticated microscopic theories. Thus, one is compelled to take recourse to construct the simplified models for describing the interaction mechanism and crystal properties. The progress model potentials have been traced in review articles written by Singh [7] and other [8, 9].

The study of dynamics of atoms in crystals is essentially a many body problem and solution of its Schrödinger's equation becomes almost impracticable due to complications in inter-atomic forces. This concept of TBI owes its origin to the non-orthogonality of the electron wave functions the first given by Lowdin [10] and Lundqvist [11]. This motives, which impelled us to undertake the present study, the successful application at three body interaction potential (TBP) [7] and acute necessity of testing its adequacies for unified description as emphasized by Cochran [8]. Later on Singh [7]. Singh and Verma [12] and their co-workers for several ionic, molecular rare gas and semiconductor solids successfully apply it. This TBP is capable to explain and Cauchy violation ( $C_{12} \neq C_{44}$ ), which is violated by experimental results in these crystals. The ionic crystals have played a very prominent part in the development of several branches of solid state physics. The estimates of the effective charges from the knowledge of observed dielectric data show a marked ionic contribution to the bonding of the solids. This ionic character is reflected by the fact that these compounds have the sodium chloride (rock salt) structure. Their partial ionic nature is also characterized by similar to the alkali halides.

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## 2. METHODS

The chalcogenide semiconductors are one farming elements. It seems to be purely ionic in nature because the constituent ions follow the additive property rule of ionic radii. The inter ionic separation ( $r_0$ ) calculated on the basis of additive property of ionic radii ( $r_0=r_+ + r_-$ ) agree well with observed values for all of them.

The ions interact with each other through long-range (LR) coulomb forces and counter balanced by the short-range (SR) repulsive forces, owing their origin to the Paul's exclusion principles. Fumi and Tosi [13] extended their BM potential by incorporating the van der Waals (vdw) interaction estimated from perturbation method of Mayer [14]. However, these models fail to explain the Cauchy discrepancy [15, 16] the phonon dispersion [17], Szigei effective charge [18] and dielectric properties [8] of crystals.

On the basis of this concept, several attempts have been made to understand the crystal interactions and some important properties, like Lattice static, dielectric, elastic, thermo physical, phase transitions or several other properties by developing several models made phenomenological and microscopic theories. Side by side theoretical investigations have also progressed and attempts have been made to understand and correlate fully the properties of these simple types of solids [19] among the crystalline crystals are marked by the fact that their constituent particles are ions carrying an integral amount of electronic charge and the electron in ions from closed shells.

A mixed crystal is made up of two chemical substances which can independently from a crystal. According to virtual crystal approximation (VCA) [20], the mixed crystals are regarded as an array of average ions whose masses, force constants and effective charge are assumed to scale linearly with concentration of host crystals.

To describe this effect the term mixed crystal is used. If the impurity ion behaves in the same charge to the Lattice ions. Wasastijerna [21] carried out a thorough study on mixed alkali halides and found that the mixed alkali halides reflected the X-rays as if they are homogeneous solutions. It should be realized that the impurity ions are all distributed randomly throughout the Lattice so that the term solid solution is more appropriate. Among mixed halides there exist wide varieties like (ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe, HgS, HgSe, and HgTe).

Chalcogenide semiconductors and its possible solid solutions which we consider for our present study are complex crystals with ZnS structure, physical and mechanical properties having electrical conductivities intermediate between metal and insulators. Certain combination from II and VI make up inter-metallic or compound semiconductors.

The present three body potential (TBP) has successfully explained both static and dynamical properties of materials with three different cubic structure, namely rock salt (RS), Cesium Chloride (CsCl) and Zinc blende (ZB) [22].

## 3. SUMMARY AND CONCLUSION

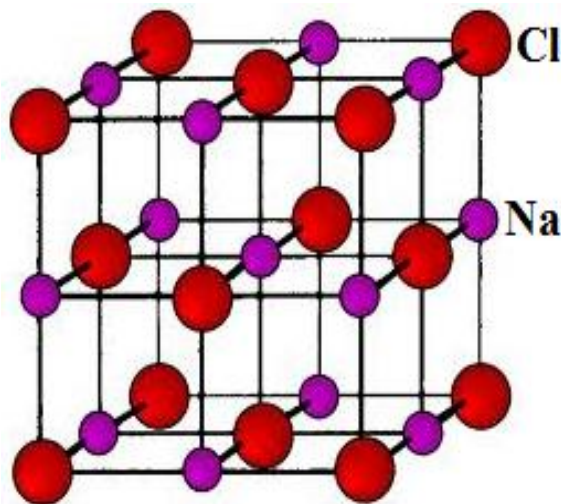
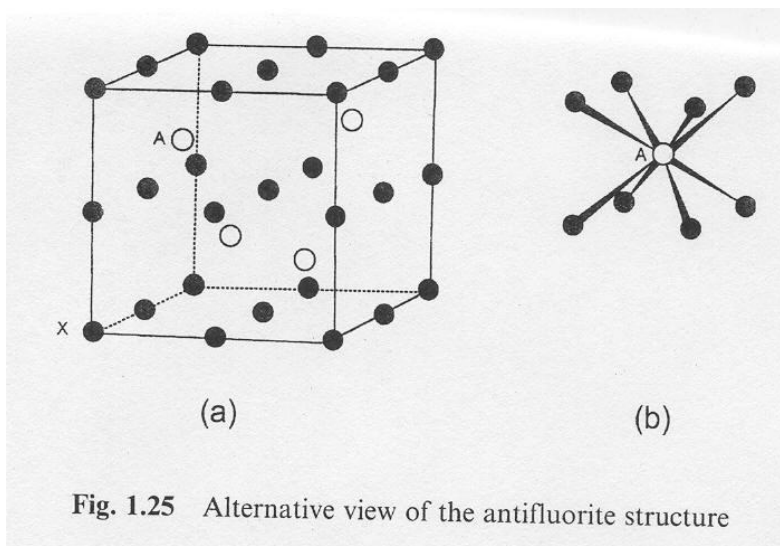


Figure 1. The rocksalt crystal structure



summarily, the structural properties of the RS structure at different pressures and temperatures are investigated. The calculated results are in excellent agreement with the available theoretical results.

Table 1. Values of Physical Constants

Solids	NaCl	CsCl	ZnS
Number of nn	6	8	4
Number of nnn	12	6	12
nn distance (r)	a	$a\sqrt{3}$	$A\sqrt{3}/2$
nnn distance (r)	$a\sqrt{3}$	2a	$2\sqrt{a}$
Cube edge	2a	2a	2a
Volume per unit cell	$2a^3$	$8a^3$	$2a^3$
Madelung constant ( $\alpha_M$ )	1.7475	1.7627	1.6381
Parameter relating r & r! (K)	$\sqrt{2}$	$2/\sqrt{3}$	$2\sqrt{2}/\sqrt{3}$

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