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## Study of crystalline structure and physical constants in solids: NaCl, CsCl, ZnS

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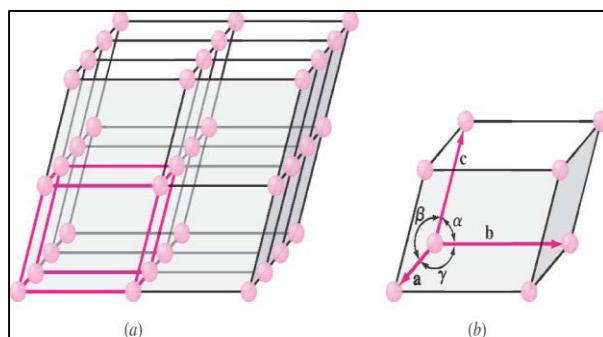
### Abstract

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. 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. In the present study crystalline structure of these materials is studied and values of different physical constants is been recorded experimentally.

**Keywords:** crystalline structure, space lattice, mixed crystal, physical constants in solids

### Introduction

The physical structure of solid materials of engineering importance depends mainly on the arrangements of the atoms, ions, or molecules that make up the solid and the bonding forces between them. If the atoms or ions of a solid are arranged in a pattern that repeats itself in three dimensions, they form a solid that is said to have a crystal structure and is referred to as a crystalline solid or crystalline material. The techniques for generating high pressure and associated measurements, described in previous chapter, have provided sufficient amount of data for the study of high-pressure behaviour of various kind of material. Atomic arrangements in crystalline solids can be described with respect to a network of lines in three dimensions. The intersections of the lines are called lattice points (or lattice sites). Each lattice point has the same environment in the same direction. A particular arrangement of atoms in a crystal structure can be described by specifying the atom positions in a repeating unit cell. The size and shape of the unit cell can be described by three lattice vectors  $a$ ,  $b$ , and  $c$ , originating from one corner of the unit cell (see Figure 1(a-b)). The axial lengths  $a$ ,  $b$ , and  $c$  and the interaxial angles  $\alpha$ ,  $\beta$ , and  $\gamma$  are the *lattice constants* of the unit cell; see Figure 1(a-b).



**Fig 1:** (a) Space lattice of ideal crystalline solid. (b) Unit cell showing lattice constants.

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Unit cells of different types can be constructed by assigning specific values for axial lengths and interaxial angles. To create all point lattices only seven different types of unit cells are necessary. These crystal systems are listed in Table-1. A number of the seven crystal systems have variations of the basic unit cell. A. J. Bravais showed that 14 standard unit cells could describe all possible lattice networks. There are four basic types of unit cells: (1) simple, (2) body-centered, (3) face-centered, and (4) base-centered. In the cubic system there are three types of unit

cells: simple cubic, body-centered cubic and face-centered cubic. In the orthorhombic system all four types are represented. In the tetragonal system there are only two: simple and body-centered. The face-centered tetragonal unit cell appears to be missing but can be constructed from four body-centered tetragonal unit cells. The monoclinic system has simple and base-centered unit cells, and the rhombohedral, hexagonal, and triclinic systems have only one simple type of unit cell.

**Table 1:** the classification of lattice space through crystal system

System	Axial lengths and interaxial angles	Space lattice
Cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	Simple Cubic Body-centered cubic Face-centered cubic
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	Simple Tetragonal Body-centered tetragonal
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	Simple Orthorhombic Body-centered orthorhombic Base-centered orthorhombic Face-centered orthorhombic
Rhombohedral	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	Simple rhombohedral
Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	Simple hexagonal
Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$	Simple monoclinic Base-centered monoclinic
Triclinic	$a \neq b \neq c, \alpha \neq \gamma \neq \beta \neq 90^\circ$	Simple triclinic

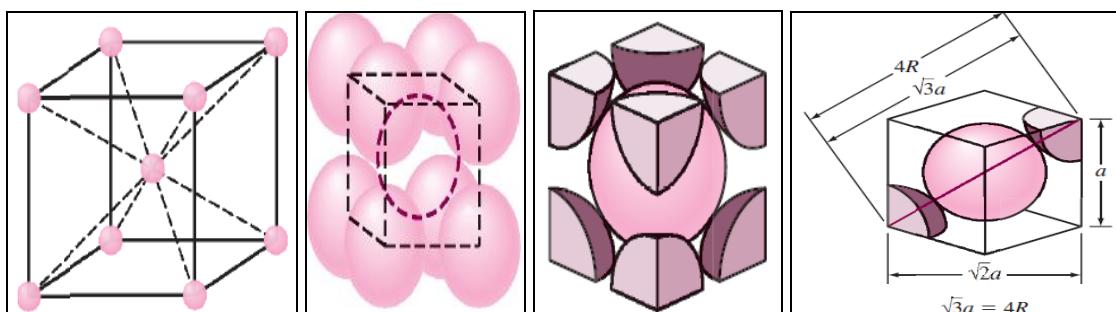
About 90% elemental metals crystallize upon solidification into three densely packed crystal structures: body-centered cubic (BCC), face-centered cubic (FCC) and hexagonal close-packed (HCP). The HCP structure is a denser modification of the simple hexagonal crystal structure. Most metals crystallize in these dense-packed structures because energy is released as the atoms come closer together and bond more tightly with each other. Thus, the densely packed structures are in lower and more stable energy arrangements.

### Body-centered cubic (BCC) crystal structure

Let us consider the atomic-site unit cell for the BCC crystal structure shown in Figure 1(a). In this unit cell the solid spheres represent the centers where atoms are located and clearly indicate their relative positions. If we represent the atoms in this cell as hard spheres, then the unit cell appears

as shown in Figure 1(b). In this unit cell we see that the central atom is surrounded by eight nearest neighbors and is said to have a coordination number of 8.

If we isolate a single hard-sphere unit cell, we obtain the model shown in Figure 1(c). Each of these cells has the equivalent of two atoms per unit cell. One complete atom is located at the center of the unit cell, and an eighth of a sphere is located at each corner of the cell, making the equivalent of another atom. Thus there is a total of 1 (at the center) +  $8 \times 1/8$  (at the corners) = 2 atoms per unit cell. The atoms in the BCC unit cell contact each other across the cube diagonal, as indicated in Figure 3(d), so that the relationship between the length of the cube side  $a$  and the atomic radius  $R$  is  $\sqrt{3}a = 4R$  or  $a = \frac{4R}{\sqrt{3}}$ . The atomic packing factor (APF) for BCC is 0.68.



**Fig 2:** For BCC(a) atomic-site unit cell, (b) hard-sphere unit cell, (c) isolated unit cell (d) BCC unit cell showing relationship between the lattice constant  $a$  and the atomic radius  $R$ .

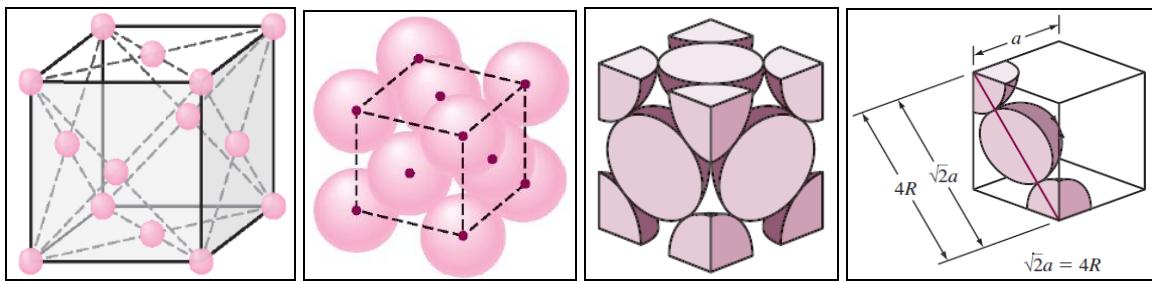
### Face-centered cubic (FCC) crystal structure

In Figure 1(a) of FCC unit cell, there is one lattice point at each corner of the cube and one at the center of each cube face. The hard-sphere model of Figure 1 (b) indicates that the atoms in the FCC crystal structure are packed as close

together as possible. The APF for this close packed structure is 0.74. The FCC unit cell as shown in Figure 1 (c) has the equivalent of four atoms per unit cell. The eight corner octants account for one atom ( $8 \times 1/8 = 1$ ), and the six half-atoms on the cube faces contribute another three atoms,

making a total of four atoms per unit cell. The atoms in the FCC unit cell contact each other across the cubic face diagonal, as indicated in Figure 3 (d), so that the relationship between the length of the cube side  $a$  and the atomic radius  $R$  is  $\sqrt{2}a = 4R$  or  $a = \frac{4R}{\sqrt{2}}$ . The APF for the FCC crystal

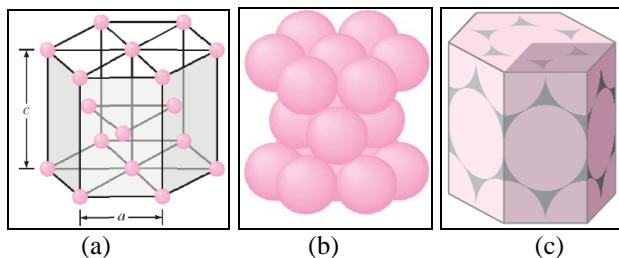
structure is 0.74, which is greater than the 0.68 factor for the BCC structure. The APF of 0.74 is for the closest packing possible of spherical atoms. Many metals such as aluminium, copper, lead, nickel, and iron at elevated temperatures crystallize with the FCC crystal structure.



**Fig 3:** For FCC (a) atomic-site unit cell, (b) hard-sphere unit cell, (c) isolated unit cell (d) FCC unit cell showing relationship between the lattice constant  $a$  and atomic radius  $R$ .

### Hexagonal closed packed (HCP) crystal structure

The HCP structure as shown in Figure 4 is the third common metallic crystal structure. Because of the very small APF metals do not crystallize into the simple hexagonal crystal structure. The atoms can attain a lower energy and a more stable condition by forming the HCP structure. The APF of the HCP crystal structure is 0.74, the same as that for the FCC crystal structure since in both structures the atoms are packed as tightly as possible. In both the HCP and FCC crystal structures each atom is surrounded by 12 other atoms and thus both structures have a coordination number of 12. The isolated HCP unit cell is shown in Figure 4 (c) and has the equivalent of six atoms per unit cell. Three atoms form a triangle in the middle layer, as indicated by the atomic sites in Figure 4 (b). There are six 1/6 atom sections on both the top and bottom layers, making an equivalent of two more atoms ( $2 \times 6 \times 1/6 = 2$ ). Finally, there is one-half of an atom in the center of both the top and bottom layers, making the equivalent of one more atom. The total number of atoms in the HCP crystal structure unit cell is thus  $3 + 2 + 1 = 6$ . The ratio of the height  $c$  of the hexagonal prism of the HCP crystal structure to its basal side  $a$  is called the *c/a ratio* (Figure 4 (a)). The *c/a ratio* for an ideal HCP crystal structure consisting of uniform spheres packed as tightly together as possible is 1.633.

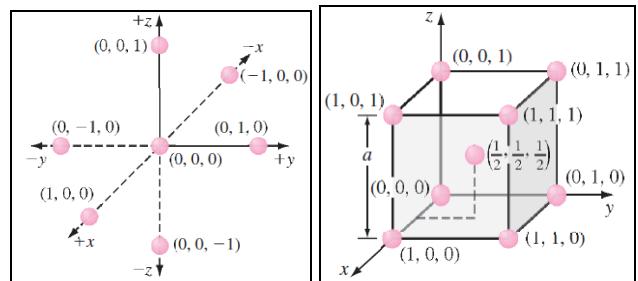


**Fig 4:** For HCP (a) atomic-site unit cell, (b) hard-sphere unit cell and (c) isolated unit cell.

### Atomic position in cubic unit cells

In cubic unit cells to locate atom positions, we use rectangular  $x$ ,  $y$ , and  $z$  axes. In crystallography the positive  $x$  axis is usually the direction coming out of the paper, the positive  $y$  axis is the direction to the right of the paper, and the positive  $z$  axis is the direction to the top (Figure 5). Negative directions are opposite to those just described. Atom positions in unit cells are located by using unit

distances along the  $x$ ,  $y$ , and  $z$  axes, as indicated in Figure 5 (a). For example, the position coordinates for the atoms in the BCC unit cell are shown in Figure 5 (b). The atomic positions for the eight corner atoms of the BCC unit cell are  $(0, 0, 0)$   $(1, 0, 0)$   $(0, 1, 0)$   $(1, 1, 0)$   $(1, 0, 1)$   $(0, 1, 1)$   $(0, 1, 1)$   $(1, 1, 1)$ . The center atom in the BCC unit cell has the position coordinates  $(1/2, 1/2, 1/2)$ . For simplicity sometimes only two atom positions in the BCC unit cell are specified which are  $(0, 0, 0)$  and  $(1/2, 1/2, 1/2)$ . The remaining atom positions of the BCC unit cell are assumed to be understood. In the same way the atom positions in the FCC unit cell can be located.



**Fig 5:** (a) Rectangular  $x$ ,  $y$ , and  $z$  axes for locating atom positions in cubic unit cells, and (b) Atom positions in a BCC unit cell.

### Zincblende (B3) structure

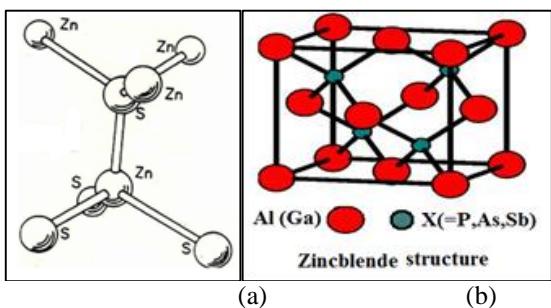
Zincblende is characterized as a cubic close packing (CCP), also known as face-centered cubic, structure as illustrated in Figure 7. The cations occupy one of the two types of tetrahedral holes present. Each atom has 4 nearest-neighbours and two different atoms per FCC lattice point. The space group of this structure is F43m (216) and strukturbericht designation is B3. Zincblende has 4 asymmetric units in its unit cell. GaAs, AlAs, GaP, GaSb, AlSb and AlP all exists in the original B3 type phase.

The choice of the primitive vectors of the Bravais face centered cubic lattice that we have adopted in this work is:  $a_1 = (0, a/2, a/2)$ ,  $a_2 = (0, 0, a/2)$ ,  $a_3 = (a/2, a/2, 0)$ ,

The position vectors of the two atoms, ( $i = 1, 2$ ), inside the unit cell, are given by

$$\mathbf{f}_1 = (0, 0, 0), \mathbf{f}_2 = (0.25a, 0.25a, 0.25a),$$

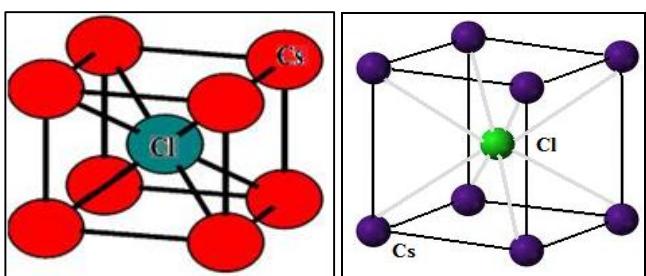
Where  $\mathbf{f}_1$  denote the vector position of the group III atoms (Ga or Al), while  $\mathbf{f}_2$  the X (=P, As, Sb) atoms.



**Fig 7:** The zincblende tetrahedral coordination with (a) two atom basis and (b) crystal structure

## Cesium Chloride (B2) (CsCl) structure

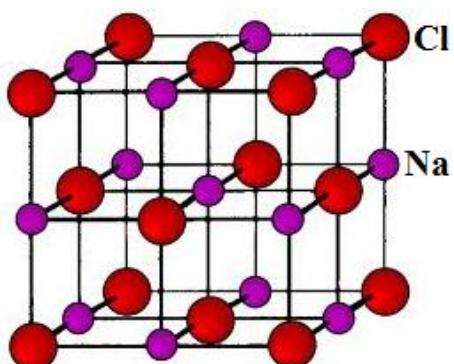
The CsCl structure is an interpenetrating primitive cubic structure each of the two different atom types forms a separate primitive cubic lattice, with an atom of one type at the center of each cube of the other type. Each atom has 8 neighbours of the opposite kind, in directions parallel to the cube body diagonal, at a distance of  $\sqrt{3} a/2$ . The space group of this structure is Pm3m (221) and strukturbericht designation is B2 (see Figure 9). The position vectors of the two atoms inside the unit cell are similar as that of rock salt structure.



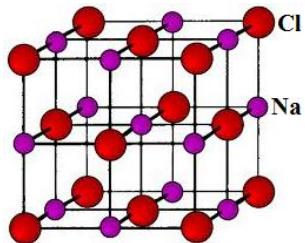
**Fig 8:** The CsCl crystal structure

## Rocksalt (B1) structure

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 B1 (see Figure 8). 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.



Anion is coordinated to 6 cations at the vertices of an octahedron.



**Fig 9:** The rocksalt crystal structure

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

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

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

### **Summary and Conclusion.**

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 interatomic 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.

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 Poul'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], Szigeti 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 caring 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).

**Table 3.1:** Values of Physical Constants

Solids	NaCl	CsCl	ZnS
Number of nn	<b>6</b>	<b>8</b>	<b>4</b>
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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