Solid State physics

Chapter One
A crystal or crystalline solid

In general solids can be divided into two distinct classes.
1) Crystalline solids
2) 2) Amorphous solids

1. *Crystal Structure.*

Lattice + Basis = crystal structure

Bravais lattice

*[Ashcroft, Kittel, J.Quinn&kyung-soo]*
<table>
<thead>
<tr>
<th>System</th>
<th>Axial lengths and angles</th>
<th>Unit cell geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>cubic</td>
<td>$a = b = c, \alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="Cubic Cell" /></td>
</tr>
<tr>
<td>tetragonal</td>
<td>$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="Tetragonal Cell" /></td>
</tr>
<tr>
<td>orthorhombic</td>
<td>$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="Orthorhombic Cell" /></td>
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<tr>
<td>rhombohedral</td>
<td>$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$</td>
<td><img src="image" alt="Rhombohedral Cell" /></td>
</tr>
<tr>
<td>hexagonal</td>
<td>$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$</td>
<td><img src="image" alt="Hexagonal Cell" /></td>
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<tr>
<td>monoclinic</td>
<td>$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$</td>
<td><img src="image" alt="Monoclinic Cell" /></td>
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<tr>
<td>triclinic</td>
<td>$a \neq b \neq c, \alpha \neq \beta \neq \gamma$</td>
<td><img src="image" alt="Triclinic Cell" /></td>
</tr>
</tbody>
</table>

*[Ashcroft, Kittel, J.Quinn&kyung-soo]*
Table 1: Geometrical characteristics of the seven crystal systems.

![Table 1: Geometrical characteristics of the seven crystal systems.](image)

Figure 1: Bravais lattices.

*Ashcroft, Kittel, J. Quinn & Kyung-soo*
1- Simple Cubic structure

The simple cubic structure has alternating atoms at each cubic lattice point.

Number of atoms per unit cell in this case = \( 8 \times \frac{1}{8} = 1 \)

2- Body Centered Cubic Unit Cell

This is a cube with an atom at each of the 8 corners, and another atom at the centre of the body diagonals.

Number of atoms per unit cell in this case = \( 8 \times \frac{1}{8} + 1 = 2 \)

3- Face Centred Cubic Unit Cell

This is a cube with an atom at each of the 8 corners, and 6 other atoms at the centre of the face diagonals.

Number of atoms per unit cell in this case

\[
= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4
\]
Coordinate NO.

Every atoms in a crystalline structure is surrounding by other atoms, by the terms **coordinate number** it mean the NO. of equidistance neighboring atoms in a given structure the coordinate NO. of each system is as follow

1- **Simple Cubic structure**

Coordinate for this case $4 + 2 = 6$ and the distance between the two nearest Niebuhr atoms = $a$.

2- **Body Centered Cubic Unit Cell**

Coordinate for this case $= 8$ and the distance between the two nearest Niebuhr atoms $= \frac{3}{2} a$

3- **Face Centred Cubic Unit Cell**

Coordinate for this case $= 12$ and the distance between the two nearest Niebuhr atoms $= a/\sqrt{2}$

**Packing Density in the Unit Cell**

When thinking of the way atoms stack together in the unit cell, it is usual to think of the atoms as solid spheres. The **packing density** refers to the fraction of space occupied by these solid spheres in their unit cell. The packing density controls the volume density of the solid and influences the way a solid either deforms plastically or fractures.

$$PF(packing\ \text{factor}) = \frac{\text{Volume of the atoms per unit cell}}{\text{volume of the unit cell}}$$

*Ashcroft, Kittel, J.Quinn&kyung-soo*
Packing density or factor for bcc

In the body centred cubic unit cell, an atom To fit the same size spheres along the body has to be at the centre of a body diagonal. If diagonal, the body diagonal must be four the atoms are taken to be all the same size, times the radius of the spheres, i.e. $d=4r$ they fit as shown below

\[ d = \sqrt{3}a = 4r \]
\[ r = \frac{\sqrt{3}}{4}a \]

Now the cube will contain the centre atom and $1/8$ of an atom from each of the 8 corner atoms, i.e. two whole atoms. The volume of two of these atoms is given by:

\[ V = 2 \times \frac{4}{3} \pi r^3 = \frac{8}{3} \pi \left(\frac{\sqrt{3}}{4}a\right)^3 \]
\[ = \frac{\sqrt{3}}{8} \pi a^3 \]
\[ = 0.68a^3 \]

The atoms occupy 68% of the cube.

Packing density or factor for fcc

In the face centred cubic unit cell, an atom To fit the same size spheres along the face has to be at the centre of a cubic face. If the diagonal, the face diagonal must be four atoms are taken to be all the same size, they times the radius of the spheres, i.e. $d=4r$

*[Ashcroft, Kittel, J.Quinn&kyung-soo]*
fit as shown below.

\[ d = \sqrt{2} a = 4r \]
\[ r = \frac{\sqrt{2}}{4} a \]

Now the cube will contain a half atom from each of the six faces and 1/8 of an atom from each of the 8 corner atoms, i.e. four whole atoms. The volume of four of these atoms is given by:

\[ V = 4 \times \frac{4}{3} \pi r^3 = \frac{16}{3} \pi \left( \frac{\sqrt{2}}{4} a \right)^3 \]
\[ = \frac{\sqrt{2}}{3} \pi a^3 \]
\[ = 0.74 a^3 \]

The atoms occupy 74% of the cube.

*[Ashcroft, Kittel, J.Quinn&kyung-soo]*
Crystal planes

Planes in a crystal can be specified using a notation called Miller indices. The Miller index is indicated by the notation [hkl] where h, k, and l are reciprocals of the plane with the x, y, and z axes. To obtain the Miller indices of a given plane requires the following steps:

1. Step 1. The plane in question is placed on a unit cell.
2. Step 2. Its intercepts with each of the crystal axes are then found.
3. Step 3. The reciprocal of the intercepts are taken.
4. Step 4. These are multiplied by a scalar to insure that is in the simple ratio of whole numbers.

For example, the face of a lattice that does not intersect the y or z axis would be (100), while a plane along the body diagonal would be the (111) plane. An illustration of this along with the (111) and (110) planes is given in Figure 2.

![Figure 2: Examples of Miller indices notation for crystal planes.](image)

*Ashcroft, Kittel, J. Quinn & Kyung-soo*
Defects in crystalline solids

Up to this point we have only been concerned with ideal structures for crystalline solids in which each atom occupies a designated point in the crystal lattice. Unfortunately, defects ordinarily exist in equilibrium between the crystal lattice and its environment. These defects are of two general types: point defects and extended defects. As their names imply, point defects are associated with a single crystal lattice site, while extended defects occur over a greater range.

Point defects: “too many or too few” or “just plain wrong”

Point defects have a significant effect on the properties of a semiconductor, so it is important to understand the classes of point defects and the characteristics of each type. Figure 3 summarizes various classes of native point defects, however, they may be divided into two general classes: defects with the wrong number of atoms (deficiency or surplus) and defects where the identity of the atoms is incorrect.

*[Ashcroft, Kittel, J. Quinn & Kyung-soo]*
Figure 3: Point defects in a crystal lattice.

[Ashcroft, Kittel, J.Quinn&kyung-soo]
Properties of crystalline solid

Crystalline solids have the following fundamentals properties.

Amorphous solds

A solid substance with its atoms held apart at equilibrium spacing, but with no long-range periodicity in atom location in its structure is an amorphous solid. Examples of amorphous solids are glass and some types of plastic. They are sometimes described as super cooled liquids because their molecules are arranged in a random manner somewhat as in the liquid state. For example, glass is commonly made from silicon dioxide or quartz sand, which has a crystalline structure.

Diffraction of X-Rays

Crystal structures are usually determined experimentally by studying how the crystal diffracts waves. Because the interatomic spacings in most crystals are of the order of a few Ås (1 Å = 10^{-8} cm), the maximum information can most readily be obtained by using waves whose wave lengths are of that