Solid State Physics-1
Crystal Structure

Dr Bindu Krishnan
What is crystal (space) lattice?

In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.
Crystal Lattice

- An infinite array of points in space,
- Each point has identical surroundings to all others.
- Arrays are arranged exactly in a periodic manner.
Crystal Structure

• Crystal structure can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sides of the lattice point.

Crystal Structure = Crystal Lattice • + Basis •
A two-dimensional Bravais lattice with different choices for the basis.
Lattice Vectors – 2D

The two vectors $a$ and $b$ form a set of lattice vectors for the lattice.

*The choice of lattice vectors is not unique.* Thus one could equally well take the vectors $a$ and $b'$ as a lattice vectors.
Lattice Vectors – 3D

An ideal three dimensional crystal is described by 3 fundamental translation vectors \(a\), \(b\) and \(c\). If there is a lattice point represented by the position vector \(r\), there is then also a lattice point represented by the position vector where \(u\), \(v\) and \(w\) are arbitrary integers.

\[
\mathbf{r}' = \mathbf{r} + u\mathbf{a} + v\mathbf{b} + w\mathbf{c}
\]  

(1)
The unit cell and, consequently, the entire lattice, is uniquely determined by the six lattice constants: \(a, b, c, \alpha, \beta\) and \(\gamma\).

- Only 1/8 of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with \(8 \times 1/8 = 1\) lattice point.
UNIT CELL

Primitive
- Single lattice point per cell
- Smallest area in 2D, or
- Smallest volume in 3D

Conventional & Non-primitive
- More than one lattice point per cell
- Integral multiples of the area of primitive cell

Simple cubic (sc)
Conventional = Primitive cell

Body centered cubic (bcc)
Conventional ≠ Primitive cell
Wigner-Seitz Method

A simply way to find the primitive cell which is called Wigner-Seitz cell can be done as follows;

1. Choose a lattice point.
2. Draw lines to connect these lattice point to its neighbours.
3. At the mid-point and normal to these lines draw new lines.

The volume enclosed is called as a Wigner-Seitz cell.
Wigner-Seitz Cell - 3D

f.c.c Wigner-Seitz cell

b.c.c Wigner-Seitz cell
Three common Unit Cell in 3D

- Simple cubic
- Body-centered cubic
- Face-centered cubic
Types Of Crystal Lattices

1) **Bravais lattice** is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed. Lattice is invariant under a translation.
2) Non-Bravais Lattice
Not only the *arrangement* but also the *orientation* must appear exactly the same from every point in a bravais lattice.

- The red side has a neighbour to its immediate left, the blue one instead has a neighbour to its right.
- Red (and blue) sides are equivalent and have the same appearance.
- Red and blue sides are not equivalent. Same appearance can be obtained rotating blue side 180°.
Five Bravais Lattices in 2D
Summary: Fourteen Bravais Lattices in Three Dimensions

The 14 possible **BRAVAISS LATTICES**

{note that spheres in this picture represent lattice points, not atoms!}

**CUBIC**
- $a = b = c$
- $\alpha = \beta = \gamma = 90^\circ$

**TETRAGONAL**
- $a = b \neq c$
- $\alpha = \beta = \gamma = 90^\circ$

**ORTHORHOMBIC**
- $a \neq b \neq c$
- $\alpha = \beta = \gamma = 90^\circ$
Fourteen Bravais Lattices...

**HEXAGONAL**
\[
a = b \neq c \\
\alpha = \beta = 90^\circ \\
\gamma = 120^\circ
\]

**MONOCLINIC**
\[
a \neq b \neq c \\
\alpha = \gamma = 90^\circ \\
\beta \neq 120^\circ
\]

**TRICLINIC**
\[
a \neq b \neq c \\
\alpha \neq \beta \neq \gamma \neq 90^\circ
\]

**TRIGONAL**
\[
a = b = c \\
\alpha = \beta = \gamma \neq 90^\circ
\]

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4 Types of Unit Cell:

- **P** = Primitive
- **I** = Body-Centred
- **F** = Face-Centred
- **C** = Side-Centred

7 Crystal Classes → 14 Bravais Lattices
Miller indices of lattice plane

- The indices of a crystal plane \((h, k, l)\) are defined to be a set of **integers** with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes:

\[
h : k : l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}
\]
001 Plane

(001) Plane referenced to the origin at point O

Other equivalent (001) planes
111 Planes

(111) Plane referenced to the origin at point $O$

Other equivalent (111) planes
110 Planes

(110) Plane referenced to the origin at point O

Other equivalent (110) planes

(b)
BCC Crystal
BCC Lattice
**Primitive and conventional cells of BCC**

Primitive Translation Vectors:

\[
\begin{align*}
\mathbf{r}_{a_1} &= \frac{1}{2}(\hat{x} + \hat{y} - \hat{z}) \\
\mathbf{r}_{a_2} &= \frac{1}{2}(-\hat{x} + \hat{y} + \hat{z}) \\
\mathbf{r}_{a_3} &= \frac{1}{2}(\hat{x} - \hat{y} + \hat{z})
\end{align*}
\]
FCC Structure
FCC lattice
Primitive and conventional cells of FCC
Hexagonal close packed cell (hcp):

conventional = primitive cell

Fractional coordinates:
100, 010, 110, 101, 011, 111, 000, 001
HCP Close Packing
When a *third layer* of spheres is placed in the indentations of the second layer there are TWO choices

- The third layer lies in indentations directly in line (*eclipsed*) with the 1st layer
  - Layer ordering may be described as *ABA*
- The third layer lies in the alternative indentations leaving it *staggered* with respect to both previous layers
  - Layer ordering may be described as *ABC*
HCP: Simple Hexagonal Bravais With Basis of Two Atoms Per Point

Figure 22  The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters $a$ and $c$ are indicated, where $a$ is in the basal plane and $c$ is the magnitude of the axis $a_3$ of Fig. 14.
Simple Crystal Structures

• There are several crystal structures of common interest: sodium chloride, cesium chloride, hexagonal close-packed, diamond and cubic zinc sulfide.

• Each of these structures have many different realizations.
NaCl Structure

1 (Sodium Chloride) Structure
CsCl Structure

B2 (CsCl) Structure
CsCl Basis
ZincBlende structure

Figure 19.4
(a) The sodium chloride structure; (b) the cesium chloride structure; (c) the zincblende (sphalerite) structure. The side of the conventional cubic cell, $a$, and the nearest-neighbor distance, $d$, are indicated in each case. Inspection of the figure reveals that they are related by: (a) sodium chloride: $d = a/2$; (b) cesium chloride: $d = \sqrt{3}a/2$; (c) zincblende: $d = \sqrt{3}a/4$. For detailed descriptions of these structures see Chapter 4.
Diamond Crystal Structure

Figure 24  Atomic positions in the cubic cell of the diamond

Figure 25  Crystal structure of diamond.
Symmetry

A state in which parts on opposite sides of a plane, line, or point display arrangements that are related to one another via a symmetry operation such as translation, rotation, reflection or inversion.

Application of the symmetry operators leaves the entire crystal unchanged.
Symmetry Elements

Inversion, or center of symmetry

Every point on one side of a center of symmetry has a similar point at an equal distance on the opposite side of the center of symmetry.
Mirror plane or Reflection

The points along the mirror line are all invariant points (points that map onto themselves) under a reflection.
Symmetry elements:
mirror plane and inversion center

Figure 3.14. The effect of a mirror and of an inversion center.

The handedness is changed.

center of symmetry
or inversion center
Rotation

Turns all the points in the asymmetric unit around one axis, the center of rotation. A rotation does not change the handedness of figures. The center of rotation is the only invariant point (point that maps onto itself).
N-fold axes with $n=5$ or $n>6$ does not occur in crystals

Adjacent spaces must be completely filled (no gaps, no overlaps).
Glide reflection (mirror plane + translation)

Reflects the asymmetric unit across a mirror and then translates parallel to the mirror. A glide plane changes the handedness of figures in the asymmetric unit. There are no invariant points (points that map onto themselves) under a glide reflection.
Screw axes (rotation + translation)

Rotation about the axis of symmetry by 360°/n, followed by a translation parallel to the axis by r/n of the unit cell length in that direction. (r < n)
Point group symmetry

• Inorganic crystals usually have perfect shape which reflects their internal symmetry
• Point groups are originally used to describe the symmetry of crystal.
• Point group symmetry does not consider translation.
• Included symmetry elements are rotation, mirror plane, center of symmetry, rotary inversion.
The combination of all available symmetry operations (32 point groups), together with translation symmetry, within the all available lattices (14 Bravais lattices) lead to 230 Space Groups that describe the only ways in which identical objects can be arranged in an infinite lattice. The International Tables list those by symbol and number, together with symmetry operators, origins, reflection conditions, and space group projection diagrams.
<table>
<thead>
<tr>
<th>Symmetry axis or symmetry point</th>
<th>Graphic symbol</th>
<th>Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis</th>
<th>Printed symbol</th>
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<td>½</td>
<td>2₁</td>
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