AIRCRAFT MATERIALS AND PROCESSES

Module - I

1. Introduction

As engineering materials constitute foundation of technology, it's not only necessary but a must to understand how materials behave like they do and why they differ in properties. This is only possible with the atomistic understanding allowed by quantum mechanics that first explained atoms and then solids starting in the 1930s. The combination of physics, chemistry, and the focus on the relationship between the properties of a material and its microstructure is the domain of Materials Science. The development of this science allowed designing materials and provided a knowledge base for the engineering applications (Materials Engineering).

Important components of the subject Materials Science are structure, properties, processing, and performance. A schematic interrelation between these four components is shown in Fig.1.

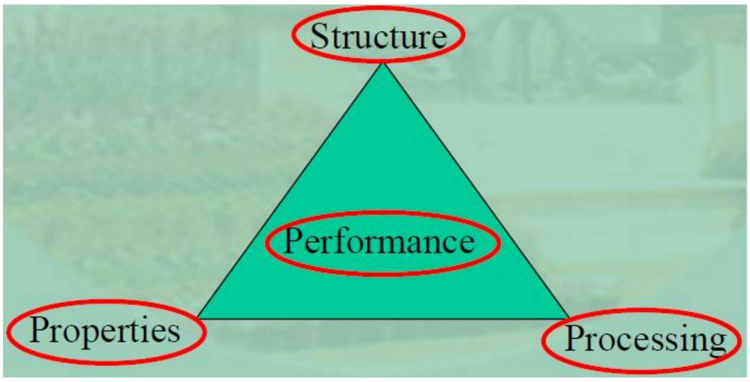

Fig.1**:** *Interrelation between four components of Materials Science.*

1.1 Classification of Materials

Like many other things, materials are classified in groups, so that our brain can handle the complexity. One can classify them based on many criteria, for example crystal structure (arrangement of atoms and bonds between them), or properties, or use. Metals, Ceramics, Polymers, Composites, Semiconductors, and Biomaterials constitute the main classes of present engineering materials.

Metals: These materials are characterized by high thermal and electrical conductivity; strong yet deformable under applied mechanical loads; opaque to light (shiny if polished). These characteristics are due to valence electrons that are detached from atoms, and spread in an *electron sea* that *glues* the ions together, i.e. atoms are bound together by metallic bonds and weaker van der Waalls forces. Pure metals are not good enough for many applications, especially structural applications. Thus metals are used in alloy form i.e. a metal mixed with another metal to improve the desired qualities. E.g.: aluminum, steel, brass, gold.

Ceramics: These are inorganic compounds, and usually made either of oxides, carbides, nitrides, or silicates of metals. Ceramics are typically partly crystalline and partly amorphous. Atoms (ions often) in ceramic materials behave mostly like either positive or negative ions, and are bound by very strong Coulomb forces between them. These materials are characterized by very high strength under compression, low ductility; usually insulators to heat and electricity. Examples: glass, porcelain, many minerals.

Polymers: Polymers in the form of thermo-plastics (nylon, polyethylene, polyvinyl chloride, rubber, etc.) consist of molecules that have covalent bonding within each molecule and van der Waals forces between them. Polymers in the form of thermo-sets (e.g., epoxy, phenolics, etc.) consist of a network of covalent bonds. They are based on H, C and other non-metallic elements. Polymers are amorphous, except for a minority of thermoplastics. Due to the kind of bonding, polymers are typically electrical and thermal insulators. However, conducting polymers can be obtained by doping, and conducting polymer-matrix composites can be obtained by the use of conducting fillers. They decompose at moderate temperatures (100 – 400 ºC), and are lightweight. Other properties vary greatly.

Composite materials: Composite materials are multiphase materials obtained by artificial combination of different materials to attain properties that the individual components cannot attain. An example is a lightweight brake disc obtained by embedding SiC particles in Al-alloy matrix. Another example is reinforced cement concrete, a structural composite obtained by combining cement (the matrix, i.e., the binder, obtained by a reaction known as hydration, between cement and water), sand (fine aggregate), gravel (coarse aggregate), and, thick steel fibers. However, there are some natural composites available in nature, for example – wood. In general, composites are classified according to their matrix materials. The main classes of composites are metal-matrix, polymer-matrix, and ceramic-matrix.

Semiconductors: Semiconductors are covalent in nature. Their atomic structure is characterized by the highest occupied energy band (the valence band, where the valence electrons reside energetically) full such that the energy gap between the top of the valence band and the bottom of the empty energy band (the conduction band) is small enough for some fraction of the valence electrons to be excited from the valence band to the conduction band by thermal, optical, or other forms of energy. Their electrical properties depend extremely strongly on minute proportions of contaminants. They are usually doped in order to enhance electrical conductivity. They are used in the form of single crystals without dislocations because grain boundaries and dislocations would degrade electrical behaviour. They are opaque to visible light but transparent to the infrared. Examples: silicon (Si), germanium (Ge), and gallium arsenide (GaAs, a compound semiconductor).

Biomaterials: These are any type material that can be used for replacement of damaged or diseased human body parts. Primary requirement of these materials is that they must be biocompatible with body tissues, and must not produce toxic substances. Other important material factors are: ability to support forces; low friction, wear, density, and cost; reproducibility. Typical applications involve heart valves, hip joints, dental implants, intraocular lenses. Examples: Stainless steel, Co-28Cr-6Mo, Ti-6Al-4V, ultra high molecular weight poly-ethylene, high purity dense Al-oxide, etc.

1.3 Advanced Materials, Future Materials, and Modern Materials needs

Advanced Materials

These are materials used in High-Tech devices those operate based on relatively intricate and sophisticated principles (e.g. computers, air/space-crafts, electronic gadgets, etc.). These materials are either traditional materials with enhanced properties or newly developed materials with high-performance capabilities. Hence these are relatively expensive. Typical applications: integrated circuits, lasers, LCDs, fiber optics, thermal protection for space shuttle, etc. Examples: Metallic foams, inter-metallic compounds, multi-component alloys, magnetic alloys, special ceramics and high temperature materials, etc.

1.3.2 Future Materials

Group of new and state-of-the-art materials now being developed, and expected to have significant influence on present-day technologies, especially in the fields of medicine, manufacturing and defense. Smart/Intelligent material system consists some type of sensor (detects an input) and an actuator (performs responsive and adaptive function). Actuators may be called upon to change shape, position, natural frequency, mechanical characteristics in response to changes in temperature, electric/magnetic fields, moisture, pH, etc.

Four types of materials used as actuators: Shape memory alloys, Piezo-electric ceramics, Magnetostrictive materials, Electro-/Magneto-rheological fluids. Materials / Devices used as sensors: Optical fibers, Piezo-electric materials, Micro-electro-mechanical systems (MEMS), etc.

Typical applications: By incorporating sensors, actuators and chip processors into system, researchers are able to stimulate biological human-like behaviour; Fibers for bridges, buildings, and wood utility poles; They also help in fast moving and accurate robot parts, high speed helicopter rotor blades; Actuators that control chatter in precision machine tools; Small microelectronic circuits in machines ranging from computers to photolithography prints; Health monitoring detecting the success or failure of a product.

1.3.3 Modern Materials

Though there has been tremendous progress over the decades in the field of materials science and engineering, innovation of new technologies, and need for better performances of existing technologies demands much more from the materials field. Moreover it is evident that new materials/technologies are needed to be environmental friendly. Some typical needs, thus, of modern materials needs are listed in the following:

- Engine efficiency increases at high temperatures: requires high temperature structural materials.
- Use of nuclear energy requires solving problem with residues, or advances in nuclear waste processing.
- Hypersonic flight requires materials that are light, strong and resist high temperatures.
- Optical communications require optical fibers that absorb light negligibly.
- Civil construction – materials for unbreakable windows.
- Structures: materials that are strong like metals and resist corrosion like plastics.

2. Atomic Structure, Interatomic Bonding and Structure of Crystalline Solids

2.1 Atomic Structure and Atomic Bonding in Solids

2.1.1 Atomic Structure

Atoms are composed of electrons, protons, and neutrons. Electrons and protons are negative and positive charged particles respectively. The magnitude of each charged particle in an atom is 1.6×10^{-19} Coulombs.

The mass of the electron is negligible with respect to those of the proton and the neutron, which form the *nucleus* of the atom. The unit of mass is an atomic mass unit (*amu*) = 1.66×10^{-27} kg, and equals 1/12 the mass of a carbon atom. The Carbon nucleus has Z=6, and A=6, where Z is the number of protons, and A the number of neutrons. Neutrons and protons have very similar masses, roughly equal to 1 *amu* each. A neutral atom has the same number of electrons and protons, Z.

A *mol* is the amount of matter that has a mass in grams equal to the atomic mass in *amu* of the atoms. Thus, a mole of carbon has a mass of 12 *grams*. The number of atoms in a mole is called the Avogadro number, $N_{av} = 6.023 \times 10^{23}$. Note that N_{av} = 1 *gram*/1 *amu*.

Calculating n, the number of atoms per cm^3 of a material of density δ (g/cm^3):

$$n = N_{av} \frac{\delta}{M}$$

where M is the atomic mass in *amu* (*grams* per *mol*). Thus, for graphite (carbon) with a density $\delta = 1.8\ g/cm^3$, M =12, we get 6×10^{23} atoms/mol × $1.8\ g/cm^3$ / 12 g/mol) = 9×10^{22} C atoms/cm^3.

For a molecular solid like ice, one uses the molecular mass, $M_{(H2O)}$ = 18. With a density of 1 g/cm^3, one obtains n = 3.3 × 10^{22} H_2O molecules/cm^3. Note that since the water molecule contains 3 atoms, this is equivalent to 9.9 × 10^{22} atoms/cm^3.

Most solids have atomic densities around 6 × 10^{22} atoms/cm^3. The cube root of that number gives the number of atoms per centimeter, about 39 million. The mean distance between atoms is the inverse of that, *or* 0.25 nm. This is an important number that gives the scale of atomic structures in solids.

2.1.2 Atomic bonding in solids

In order to understand the why materials behave like they do and why they differ in properties, it is necessary that one should look at atomic level. The study primarily concentrates on two issues: what made the atoms to cluster together, and how atoms are arranged. As mentioned in earlier chapter, atoms are bound to each other by number of bonds. These inter-atomic bonds are primarily of two kinds: Primary bonds and Secondary bonds. Ionic, Covalent and Metallic bonds are relatively very strong, and grouped as primary bonds, whereas van der Waals and hydrogen bonds are relatively weak, and termed as secondary bonds. Metals and Ceramics are entirely held together by primary bonds - the ionic and covalent bonds in ceramics, and the metallic and covalent bonds in metals. Although much weaker than primary bonds, secondary bonds are still very important. They provide the links between polymer molecules in polyethylene (and other polymers) which make them solids. Without them, water would boil at -80°C, and life as we know it on earth would not exist.

Ionic Bonding: This bond exists between two atoms when one of the atoms is negative (has an extra electron) and another is positive (has lost an electron). Then there is a strong, direct Coulomb attraction. Basically ionic bonds are non-directional in nature. An example is NaCl. In the molecule, there are more electrons around Cl, forming Cl^- and fewer electrons around Na, forming Na^+. Ionic bonds are the strongest bonds. In real solids, ionic bonding is usually exists along with covalent bonding.

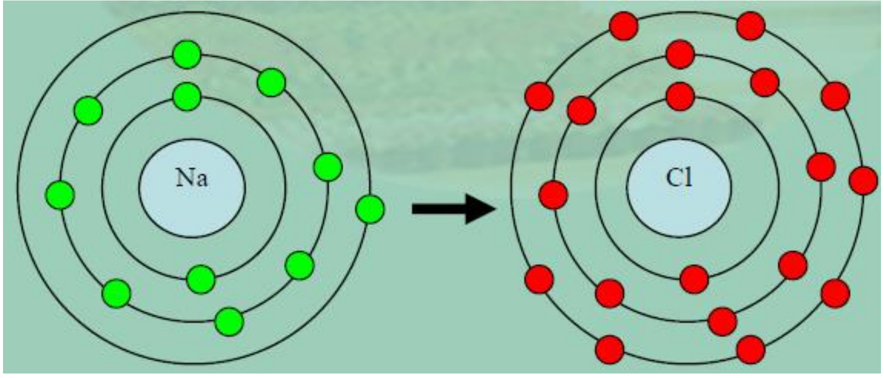

Fig.2 : Schematic representation of ioning bonding. Here, Na is giving an electron to Cl to have stable structure

Covalent Bonding: In covalent bonding, electrons are shared between the atoms, to saturate the valency. The simplest example is the H_2 molecule, where the electrons spend more time in between the nuclei of two atoms than outside, thus producing bonding. Covalent bonds are stereo-specific i.e. each bond is between a specific pair of atoms, which share a pair of electrons (of opposite magnetic spins). Typically, covalent bonds are very strong, and directional in nature. The hardness of diamond is a result of the fact that each carbon atom is covalently bonded with four neighbouring atoms, and each neighbour is bonded with an equal number of atoms to form a rigid three-dimensional structure.

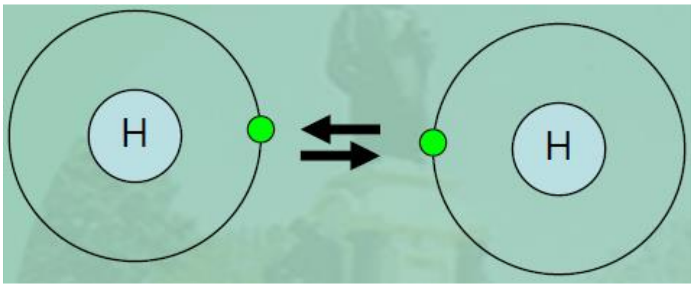

Fig. 3 : Schematic representation of covalent bond in Hydrogen molecule (sharing of electrons)

Metallic Bonding: Metals are characterized by high thermal and electrical conductivities. Thus, neither covalent nor ionic bondings are realized because both types of bonding localize the valence electrons and preclude conduction. However, strong bonding does occur in metals. The valence electrons of metals also are delocalized. Thus metallic bonding can be viewed as metal containing a periodic structure of positive ions surrounded by a sea of delocalized electrons. The attraction between the two provides the bond, which is non-directional.

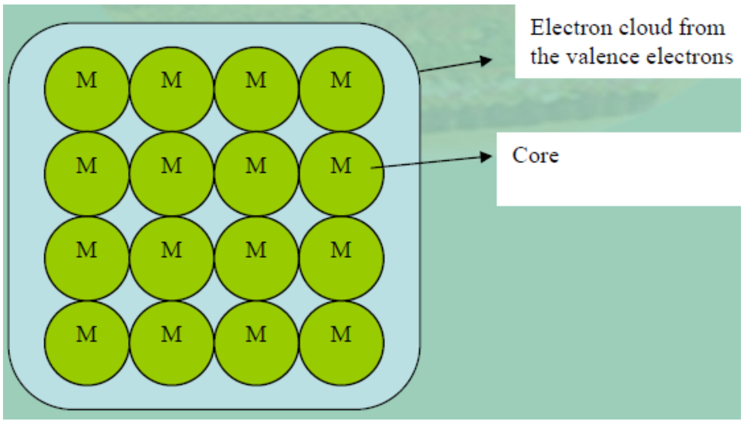

Fig. 4: Metallic bonding.

Fluctuating Induced Dipole Bonds: Since the electrons may be on one side of the atom or the other, a dipole is formed: the + nucleus at the center, and the electron outside. Since the electron moves, the dipole fluctuates. This fluctuation in atom A produces a fluctuating electric field that is felt by the electrons of an adjacent atom, B. Atom B then polarizes so that its outer electrons are on the side of the atom closest to the + side (or opposite to the – side) of the dipole in A.

Polar Molecule-Induced Dipole Bonds: Another type of secondary bond exists with asymmetric molecules, also called polar molecules because of positively and negatively charged regions. A permanent dipole moment arises from net positive and negative charges that are respectively associated with the hydrogen and chlorine ends of the HCl molecule, leading to bonding. The magnitude of this bond will be greater than for fluctuating induced dipoles.

These two kinds of bonds are also called van der Waals bonds. Third type of secondary bond is the hydrogen bond. It is categorized separately because it produces the strongest forces of attraction in this category.

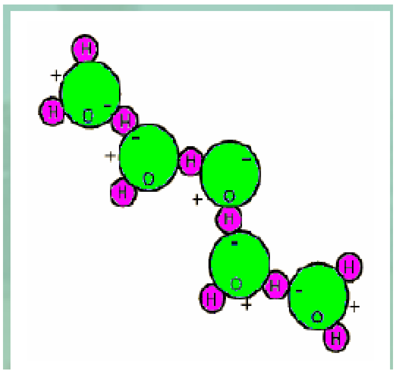

Fig. 5: Dipole bond in water

Permanent Dipole Bonds / Hydrogen bonding: It occurs between molecules as covalently bonded hydrogen atoms – for example C-H, O-H, F-H – share single electron with other atom essentially resulting in positively charged proton that is not shielded any electrons. This highly positively charged end of the molecule is capable of strong attractive force with the negative end of an adjacent molecule. The properties of water are influenced significantly by the hydrogen bonds/bridges. The bridges are of sufficient strength, and as a consequence water has the highest melting point of any molecule of its size. Likewise, its heat of vaporization is very high.

2.2 Crystal Structures, Crystalline and Non-Crystalline materials

2.2.1 Crystal structures

All metals, a major fraction of ceramics, and certain polymers acquire crystalline form when solidify, i.e. in solid state atoms self-organize to form *crystals*. Crystals possess a long-range order of atomic arrangement through repeated periodicity at regular intervals in three dimensions of space. When the solid is not crystalline, it is called amorphous. Examples of crystalline solids are metals, diamond and other precious stones, ice, graphite. Examples of amorphous solids are glass, amorphous carbon (a-C), amorphous Si, most plastics.

There is very large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex structures for ceramics and some polymers. To discuss crystalline structures it is useful to consider atoms as being hard spheres, with well-defined radii. In this scheme, the shortest distance between two like atoms is one diameter. In this context, use of terms *lattice* and *unit cell* will be handy. *Lattice* is used to represent a three-dimensional periodic array of points coinciding with atom positions. *Unit cell* is smallest repeatable entity that can be used to completely represent a crystal structure. Thus it can be considered that a unit cell is the building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.

Important properties of the unit cells are

- The type of atoms and their radii R.
- Cell dimensions (Lattice spacing a, b and c) in terms of R and
- Angle between the axis α, β, γ
- a*, b*, c* - lattice distances in reciprocal lattice , α^*, β^*, γ^* - angle in reciprocal lattice
- n, number of atoms per unit cell. For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, $1/m$.
- CN, the coordination number, which is the number of closest neighbours to which an atom is bonded.
- APF, the atomic packing factor, which is the fraction of the volume of the cell actually occupied by the hard spheres. APF = Sum of atomic volumes/Volume of cell.

Some very common crystal structures and relevant properties are listed in table 1.

Table 1: Common crystal structures and their properties.

Unit Cell	*n*	*CN*	*a*/*R*	*APF*
Simple Cubic	1	6	4/√4	0.52
Body-Centered Cubic	2	8	4/√ 3	0.68
Face-Centered Cubic	4	12	4/√ 2	0.74
Hexagonal Close Packed	6	12		0.74

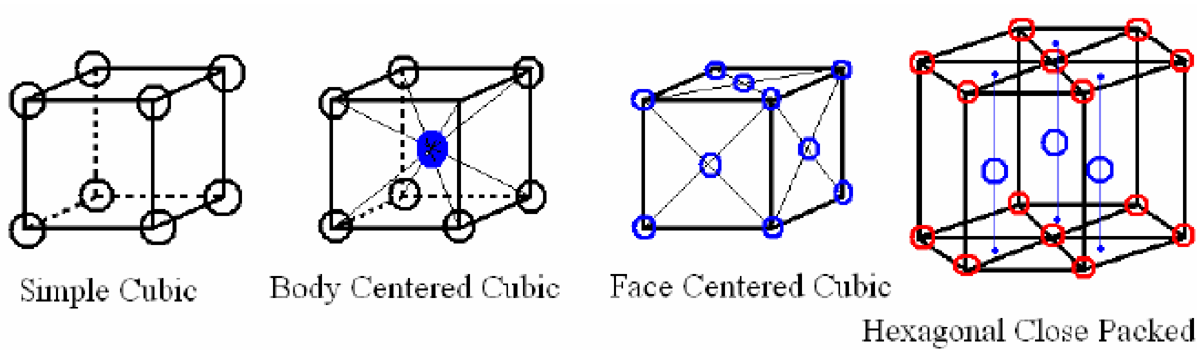

Fig. 6: Common metallic crystal structures.

2.2.2 Crystalline and Non-crystalline materials

Single Crystals: Crystals can be *single crystals* where the whole solid is one crystal. Then it has a regular geometric structure with flat faces.

Polycrystalline Materials: A solid can be composed of many crystalline grains, not aligned with each other. It is called *polycrystalline*. The grains can be more or less aligned with respect to each other. Where they meet is called a *grain boundary*.

Non-Crystalline Solids: In amorphous solids, there is no long-range order. But amorphous does not mean random, since the distance between atoms cannot be smaller than the size of the hard spheres. Also, in many cases there is some form of short-range order. For instance, the tetragonal order of crystalline SiO_2 (quartz) is still apparent in amorphous SiO_2 (silica glass).

2.3 Miller Indices, Anisotropy, and Elastic behaviour of composites

2.3.1 Miller indices:

It is understood that properties of materials depend on their crystal structure, and many of these properties are directional in nature. For example: elastic modulus of BCC iron is greater parallel to the body diagonal than it is to the cube edge. Thus it is necessary to characterize the crystal to identify specific directions and planes. Specific methods are employed to define crystal directions and crystal planes.

Methodology to define crystallographic directions in cubic crystal:

- a vector of convenient length is placed parallel to the required direction.
- the length of the vector projection on each of three axes are measured in unit cell dimensions.
- these three numbers are made to smallest integer values, known as indices, by multiplying or dividing by a common factor.
- the three indices are enclosed in square brackets, *[uvw]*. A family of directions is represented by <*uvw*>.

Methodology to define crystallographic planes in cubic crystal:

- determine the intercepts of the plane along the crystallographic axes, *in terms of unit cell dimensions*. If plane is passing through origin, there is a need to construct a plane parallel to original plane.
- take the reciprocals of these intercept numbers.
- clear fractions.
- reduce to set of smallest integers.
- The three indices are enclosed in parenthesis, *(hkl)*. A family of planes is represented by *{hkl}*.

For example, if the x-, y-, and z- intercepts of a plane are 2, 1, and 3. The Miller indices are calculated as:

- take reciprocals: 1/2, 1/1, 1/3.
- clear fractions (multiply by 6): 3, 6, 2.
- reduce to lowest terms (already there). => Miller indices of the plane are (362).

Fig. 7 depicts Miller indices for number of directions and planes in a cubic crystal.

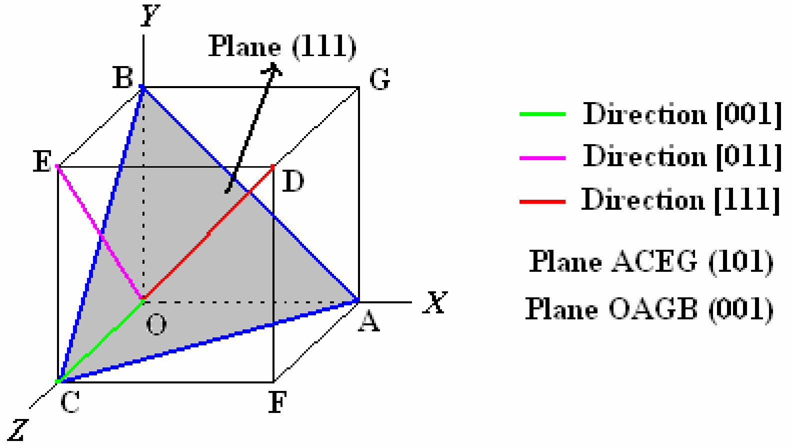

Fig. 7: *Miller indices in a cubic crystal.*

Some useful conventions of Miller notation:

- If a plane is parallel to an axis, its intercept is at infinity and its Miller index will be zero.
- If a plane has negative intercept, the negative number is denoted by a bar above the number. *Never alter negative numbers.* For example, do not divide -1, -1, -1 by -1 to get 1,1,1. This implies symmetry that the crystal may not have!
- The crystal directions of a family are not necessarily parallel to each other. Similarly, not all planes of a family are parallel to each other.
- By changing signs of all indices of a direction, we obtain opposite direction. Similarly, by changing all signs of a plane, a plane at same distance in other side of the origin can be obtained.
- Multiplying or dividing a Miller index by constant has no effect on the orientation of the plane.
- The smaller the Miller index, more nearly parallel the plane to that axis, and vice versa.
- When the integers used in the Miller indices contain more than one digit, the indices must be separated by commas. E.g.: (3,10,13)
- By changing the signs of all the indices of (a) a direction, we obtain opposite direction, and (b) a plane, we obtain a plane located at the same distance on the other side of the origin.

More conventions applicable to cubic crystals only:

- [*uvw*] is normal to (*hkl*) if $u = h$, $v = k$, and $w = l$. E.g.: (111) $\perp$ [111].
- Inter-planar distance between family of planes {*hkl*} is given by:

$$d_{\{hkl\}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

- [*uvw*] is parallel to (*hkl*) if $hu + kv + lw = 0$.
- Two planes ($h_1k_1l_1$) and ($h_2k_2l_2$) are normal if $h_1h_2 + k_1k_2 + l_1l_2=0$.
- Two directions ($u_1v_1w_1$) and ($u_2v_2w_2$) are normal if $u_1u_2 + v_1v_2 + w_1w_2=0$
- Angle between two planes is given by:

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

The same equation applies for two directions.

Why Miller indices are calculated in that way?

- Using reciprocals spares us the complication of infinite intercepts.
- Formulas involving Miller indices are very similar to related formulas from analytical geometry.
- Specifying dimensions in unit cell terms means that the same label can be applied to any plane with a similar stacking pattern, regardless of the crystal class of the crystal. Plane (111) always steps the same way regardless of crystal system.

Determination of Crystal Structure by X-RAY Diffraction

X-rays provide a powerful tool for the study of crystal structure. X-rays, being electromagnetic radiations, also undergo the phenomenon of diffraction as observed for visible light. The ordered arrangement of atoms in a crystal with interatomic spacing of the order of few angstroms behaves like a three-dimensional diffraction grating for X-rays. One can easily verify this. Let us consider sodium metal whose density ρ and molecular weight, M are 1.013×10^3 kg/m^3 and 23 respectively. The structure of sodium is BCC and number of atoms/unit volume = $N\rho/M = 2/a^3$, where N is Avogadro number (= 6.023×10^{26}) and a is cell constant. So, we have

$$a = \left(\frac{2M}{N\rho}\right)^{1/3} = \left[\frac{2 \times 23}{6.023 \times 10^{26} \times 1.013 \times 10^3}\right]^{1/3} = 4.225\ \text{Å}$$

Thus the wavelength of the radiation required for diffraction by sodium metal is of the order of a few angstroms which is clearly in the range of X-rays. We can easily show that the required voltage in the X-ray tube to produce this wavelength is 10 – 50 keV.

Bragg's Law of X-ray Diffraction

In 1912, Laue suggested that a crystal which consisted of a three-dimensional array of regularly spaced atoms could serve as a grating. The crystal differs from the ordinary grating in the sense that the diffracting centres in the crystal are not in one plane, i.e. crystal acts as a space grating rather than plane grating used for the study of light diffraction.

On the suggestion of Laue, his associates succeeded in diffracting X-rays by passing them through a thin crystal of Zinc blende. The diffraction pattern obtained by them consists of a central spot and a series of spots arranged in a definite pattern around the central spot. This symmetrical pattern of spots is known as Laue pattern. The explanation for this was given by Bragg. According to Bragg, the spots are produced due to the reflection of some of the incident X-rays from the various sets of parallel crystal planes (called as Bragg's planes), which contain a large number of atoms.

Consider a ray PA reflected at atom A in the direction AR from plane I and another ray QB reflected at another atom B in the direction BS (Fig. 3.63). Now, draw two perpendiculars AC and AD from the atom A on QB and BS respectively. The two reflected rays AR and BS will be in phase or out of phase depending on the path difference. When the path difference, $CB + BD$ is a whole wavelength λ, or multiple of whole wavelength ($n\lambda$), then the two rays will reinforce each other and produce an intense spot due to constructive interference. Obviously, the condition of reinforcement, i.e. constructive interference is:

$$CB + BD = n\lambda$$

$$CB = BD = d \sin \theta$$

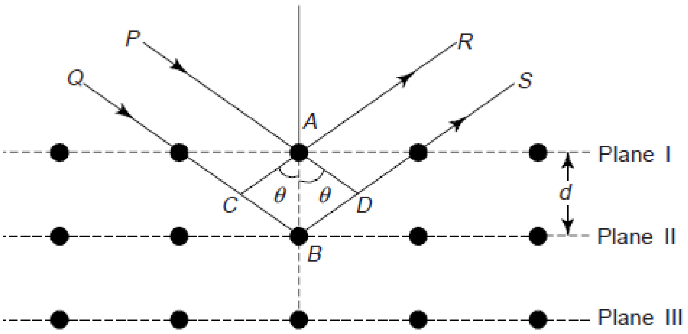

Fig. 3.63 Reflection of X-rays from lattice planes in a crystal and derivation of Bragg's law

where, θ is the angle between the incident ray and the planes of reflection and called as *glancing angle*. Therefore, we have

$$2d \sin \theta = n\lambda \tag{11}$$

where d is the interplanar spacing of planes, i.e. distance between the same set of planes and $n = 1, 2, 3, \ldots$ stand for first order, second order, third order maxima respectively. Equation (11) is known as Bragg's law. We must note that the Bragg's reflection can occur only for $\lambda \leq 2d$.

The directions along which the maxima are observed can be obtained from Bragg's law, by giving different values of θ, i.e.,

for first maximum, $\sin \theta_1 = \dfrac{\lambda}{2d}$

for second maximum, $\sin \theta_2 = \dfrac{2\lambda}{2d}$

for third maximum, $\sin \theta_3 = \dfrac{3\lambda}{2d}$ and so on.

. . . .

As the order of spectrum increases, the intensity goes on decreasing.

We must note that the Bragg equation is not limited to atomic planes parallel to the crystal surface. Sets of parallel atomic planes can be constructed through the crystal at different angles. The value of the grating space d is different for each set of parallel planes.

Reflection rules of X-ray diffraction for common metal structures are summarized in the following table 3.3

Table 3.3 Reflection rules of X-ray diffraction for the common metal structures

Crystal structure	*Diffraction does not occur for*	*Diffraction occurs for*
BCC	$h + k + l$ = odd number	$h + k + l$ = even number
FCC	h, k, l can have both even and odd integer values	h, k, l can be all even or all odd numbers
HCP	$h + 2k = 3n$, l odd ($n \rightarrow$ integer)	All other cases

29. BRAGG'S X-RAY SPECTROMETER

The X-rays from the target *T* of an X-ray tube pass through two slits S_1 and S_2 in thick lead sheets (Fig. 3.64). They then fall on the single crystal *D* mounted on a turn table. The crystal is rotated by means of the turn-table so as to increase the glancing angle at which X-rays are incident at the exposed face of the crystal. The position of the crystal can be read with the help of the vernier *v* and *a* circular scale. An ionisation chamber *I* is mounted on an arm which can rotate about the same axis as that of the crystal table. The ionisation chamber or photographic plate is used for measuring the intensities of reflected rays. The angles, for which reflection intensities are maximum, give the values of θ of equation $n\lambda = 2d \sin \theta$. One can carry out the process for each plane of the crystal. $n = 1$ creates the condition for the lowest angle at which the lowest reflection occurs. $n = 2$ creates the condition for the next higher angle at which the maximum reflection occurs and so on. Thus, we have

For $n = 1$ $\quad \lambda = 2d \sin \theta_1$

$n = 2$ $\quad 2\lambda = 2d \sin \theta_2$,

$n = 3$ $\quad 3\lambda = 2d \sin \theta_3$, etc.

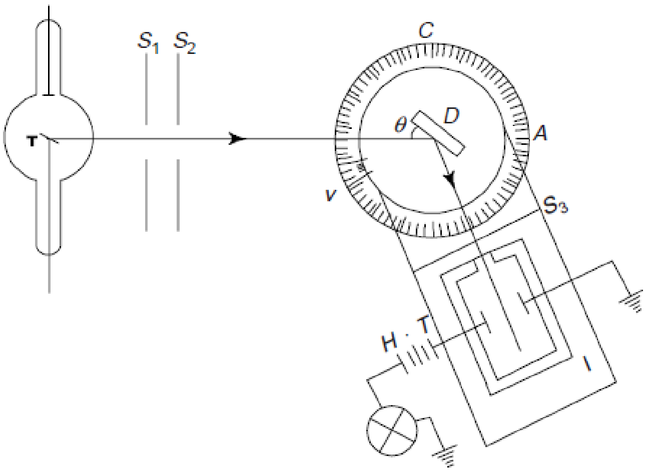

Fig. 3.64 Bragg's X-ray spectrometer

where θ_1, θ_2 and θ_3 are glancing angles for $n = 1$, 2 and 3 respectively. Thus

$$\sin \theta_1 : \sin \theta_2 : \sin \theta_3 = 1 : 2 : 3 \tag{12}$$

Obviously, by measuring glancing angles at which reflection occurs, one can determine the interplanar spacings knowing the wavelength of X-rays.

The variation of ionization current against glancing angle θ is shown in Fig. 3.65. This curve is obtained when X-rays from a tube containing a platinum target were reflected by a crystal of rock salt (NaCl).

The experimental results have shown that the first order reflection maxima occurred at 5.9°, 8.4° and 5.2° for (100), (110) and (111) planes respectively.

For first order reflection, $n = 1$ and hence

$$d = \frac{\lambda}{2 \sin \theta}$$

or

$$d \propto \frac{1}{\sin \theta}$$

$$\therefore \quad d_{100} : d_{110} : d_{111} = \frac{1}{\sin \theta_1} : \frac{1}{\sin \theta_2} : \frac{1}{\sin \theta_3}$$

or

$$d_{100} : d_{110} : d_{111} = \frac{1}{\sin 5.9^\circ} : \frac{1}{\sin 8.4^\circ} : \frac{1}{\sin 5.2^\circ}$$

$$= 9.73 : 6.84 : 11.04$$

$$\therefore \quad d_{100} : d_{110} : d_{111} = 1 : \frac{1}{\sqrt{2}} : \frac{2}{\sqrt{3}}$$

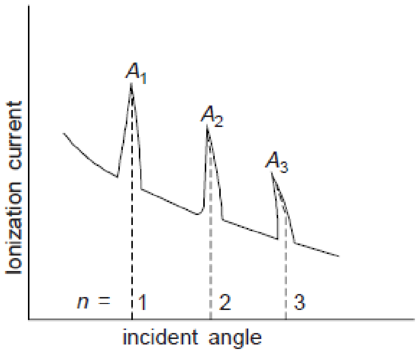

Fig. 3.65 Variation of ionization current with glancing angle

One can follow this procedure for other crystals. Following table summarizes the values of ratios between interplanar distance of planes (100), (110) and (111) for the cubic structures.

Table 3.4 Ratio between interplanar distances

S. No.	*Type of cubic structure*	$\frac{1}{d_{100}}$	:	$\frac{1}{d_{110}}$	:	$\frac{1}{d_{111}}$
1	Simple cubic	1	:	$\sqrt{2}$	:	$\sqrt{3}$
2	BCC	1	:	$\frac{1}{\sqrt{2}}$	:	$\sqrt{3}$
3	FCC	1	:	$\sqrt{2}$	:	$\frac{\sqrt{3}}{2}$

Example 25 *Determine the interplanar spacing when a beam of X-ray of wavelength 1.54 Å is directed towards the crystal at angle 20.3° to the atomic plane.* [AMIE]

Solution $2d \sin \theta = n\lambda$ | $\lambda = 1.54$ Å

∴ $2d \sin 20.3° = 1 \times 1.54$ | $\theta = 20.3°$

$$\therefore \qquad d = \frac{1.54}{2 \sin 20.3°} = \frac{1.54}{2 \times 0.3469} = 2.22 \text{ Å}$$

Example 26 *X-rays with wavelength of 0.58 Å are used for calculating d_{200} in nickel. The reflection angle is 9.5°. What is the size of unit cell?* [AMIE]

Solution $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$ | $\lambda = 0.58$ Å

$\theta = 9.5°$

$$\therefore \qquad d_{200} = \frac{a}{\sqrt{2^2 + 0^2 + 0^2}} = \frac{a}{2} = 0.5a$$

Now, from Bragg's law

$2d \sin \theta = n\lambda$, we have

$$2\, d_{200} \sin 9.5° = 1 \times 0.58$$

$$2 \times 0.5a \times 0.165 = 0.58$$

$$\therefore \qquad a = \frac{0.58}{1.165} = 0.52 \text{ Å}$$

Example 27 *Calculate the Bragg angle if (111) planes of a cube (a = 3.57 Å) crystal are exposed to X-rays (wavelength = 1.54 Å)* [AMIE]

Solution We have, Miller indices of the (111) planes, $h = 1$, $k = 1$ and $l = 1$; $a = 3.57°$ and $\lambda = 1.54$ Å. Let θ be the Bragg's angle for the first order reflection.

We have $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$d_{111} = \frac{3.57}{\sqrt{(1)^2 + (1)^2 + (1)^2}} = 2.06 \text{ Å}$$

Now, from Bragg's law, we have

$$2d_{111} \sin \theta = n\lambda$$

$$\therefore \qquad 2 \times 2.06 \times \sin \theta = 1 \times 0.54$$

$$\sin \theta = \frac{1 \times 0.54}{2 \times 2.06} = 0.131$$

$$\theta = 7° \; 32'$$

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