

Electrical Materials Code-5EE3-01

Unit -2

BONDING IN SOLIDS

A comprehension of a large number of the physical properties of materials is predicated on information of the nuclear powers that quarry the particles together. Maybe the standards of nuclear holding are best represented by considering the connection between two confined particles as they are brought into closeness from an interminable division. Everywhere the connections are insignificant, however as the molecules approach, each repels the other. These powers are of two sorts, alluring and appalling, and the greatness of each is an element of the detachment or interatomic separation.

The orbit of an alluring power F_A relies on the specific kind of holding that exists between the two molecules. The size of the alluring power shifts with the separation, as shown schematically in Figure 2.7a. At last, the external electron shells of the two atoms start to cover, and a solid shocking power F_R becomes possibly the most important factor. The net compel F_N between the two molecules is only the total of both alluring and terrible parts; that is,

$$F_N = F_R + F_A$$

Three unique sorts of primary or chemical bond are found in solids—ionic, covalent, and metallic. For every sort, the holding essentially includes the valence electrons; moreover, the nature of the bond relies on the electron structures of the constituent molecules. By and large, each of these three sorts of holding emerges from the inclination of the molecules to expect stable electron structures, similar to those of the inactive gasses, by totally filling the furthest electron shell. Auxiliary or physical strengths and energies are likewise found in numerous strong materials; they are weaker than the essential ones, yet regardless impact the physical properties of a few materials. The segments that take after clarify the few sorts of essential and auxiliary between nuclear or atomic bonds.

Primary Interatomic Bonds

Ionic Bonds: Ionic bonding may be the least demanding to depict and picture. It is constantly found in abundance that are made out of both metallic and non-metallic elements. Elements that are arranged at the flat limits of the occasional table. Molecules of a metallic element effortlessly surrender their valence electrons to the non-metallic atoms. In the process every one of the molecules procures steady or inactive gas setups and, furthermore, an electrical charge; that is, they get particles. Sodium chloride (NaCl) is an exemplary ionic material. A sodium molecule can accept the electron structure of neon (and a net single positive charge) by an exchange of its one valence $3s$ electron to a chlorine particle. After such an exchange, the chlorine particle has a net negative charge and an electron setup indistinguishable to that of argon. In sodium chloride, all the

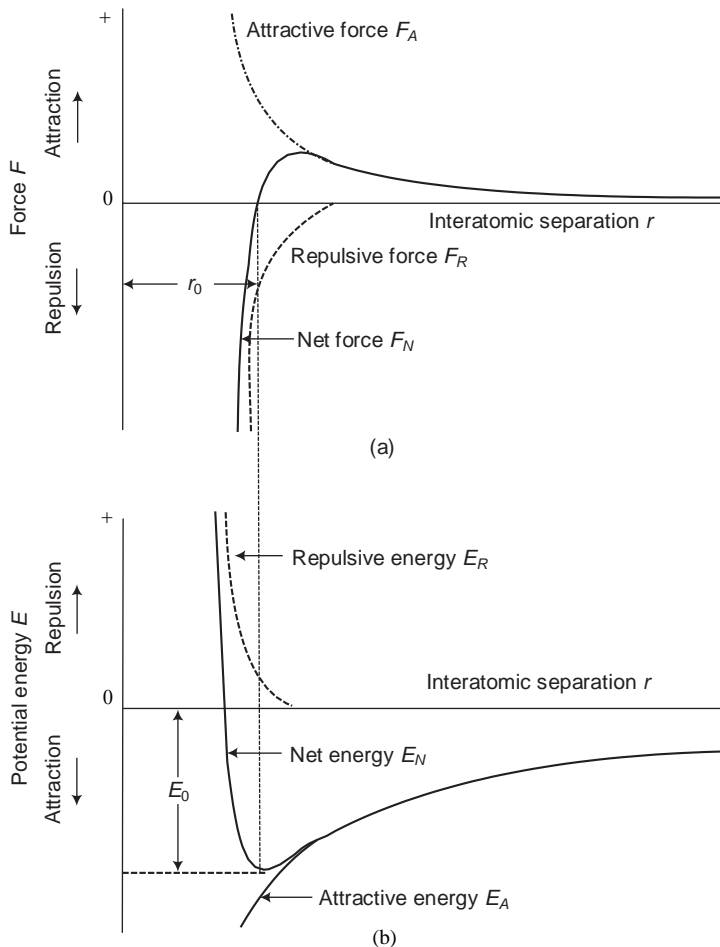


Figure: The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms. (b) The dependence of repulsive, attractive, and net potential energies on inter-atomic separation for two isolated atoms.

sodium and chlorine exist as particles. This sort of holding is shown schematically in Figure 2.8.

Hence, we can summarize that this bond exists between two atoms when one of the atoms is negative (has an additional electron) and another is positive (has lost an electron). At that point there is a solid, coordinate Coulomb fascination. Essentially, ionic bonds are non-directional in nature. An illustration is NaCl. In the particle, there are more electrons around Cl, shaping Cl^- and less electrons around Na, framing Na^+ . Ionic bonds are the most grounded bonds. In genuine solids, ionic holding typically exists alongside covalent holding.

Covalent Bonds: In covalent bonding, stable electron setups are expected by the sharing of electrons between neighbouring atoms. Two atoms that are covalently fortified will each contribute no less than one electron to the bond, and the mutual electrons might be considered to have a place with both particles. Covalent holding is schematically delineated in Figure 2.9 for an atom of methane (CH_4). The carbon particle has four valence electrons, though each of the four hydrogen molecules has a solitary valence electron. Every hydrogen iota can obtain a helium electron arrangement (two 1s valence electrons) when the carbon molecule offers with it one electron. Carbon now has four extra shared electrons, one from every hydrogen, for an aggregate of eight valence electrons, and the electron structure of neon. The covalent bond is directional; that is, it is between particular particles and may exist just in the course between one iota and another that takes part in the electron sharing.

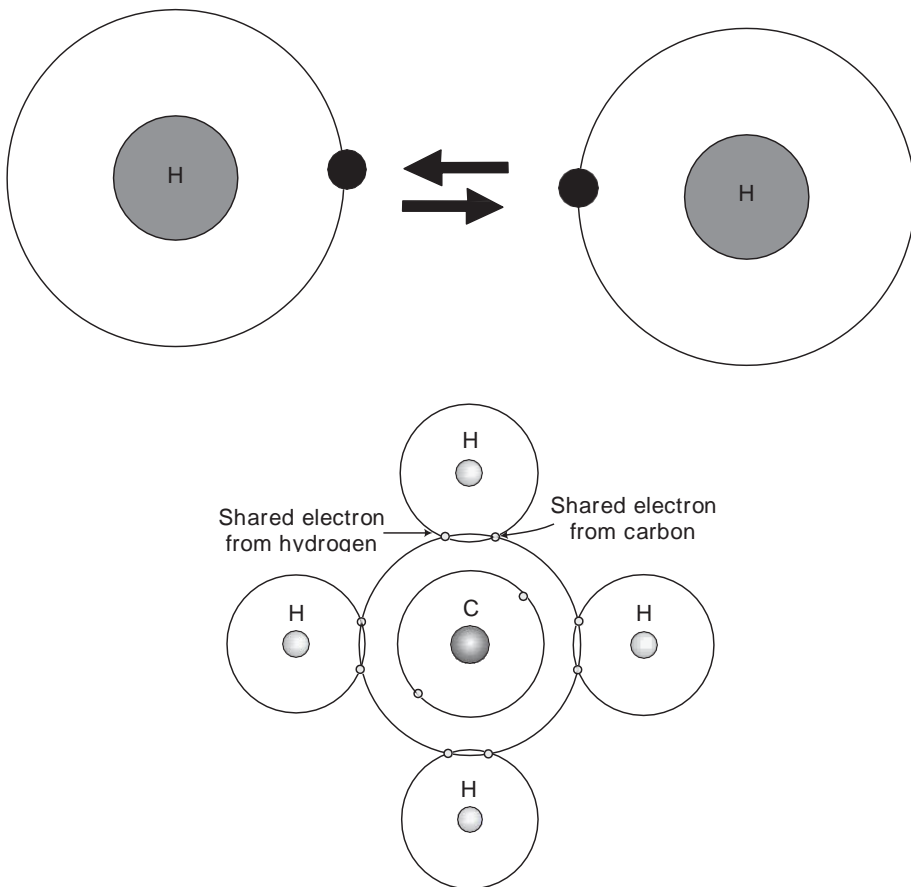


Figure: Schematic representation of a covalent bond in hydrogen molecule (sharing of electrons).

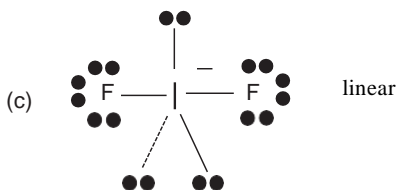
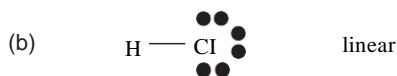
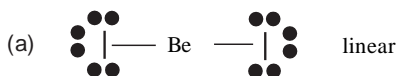
Hence, we can summarize covalent bonding that in this type of bonding electrons are shared between the atoms, to soak the valency. The most straightforward case is the H_2 particle, where the electrons invest more energy in the middle of the cores of two atoms than outside, along these lines delivering holding. Covalent bonds are stereo- particular, i.e., every bond is between a particular match of particles, which share a couple of electrons (of inverse attractive twists). Regularly, covalent bonds are exceptionally solid, and directional in nature. The hardness of precious stone is an after- effect of the way that every carbon molecule is covalently reinforced with four neighbouring particles, and every neighbour is fortified with an equivalent number of atoms to shape an inflexible three-dimensional structure.

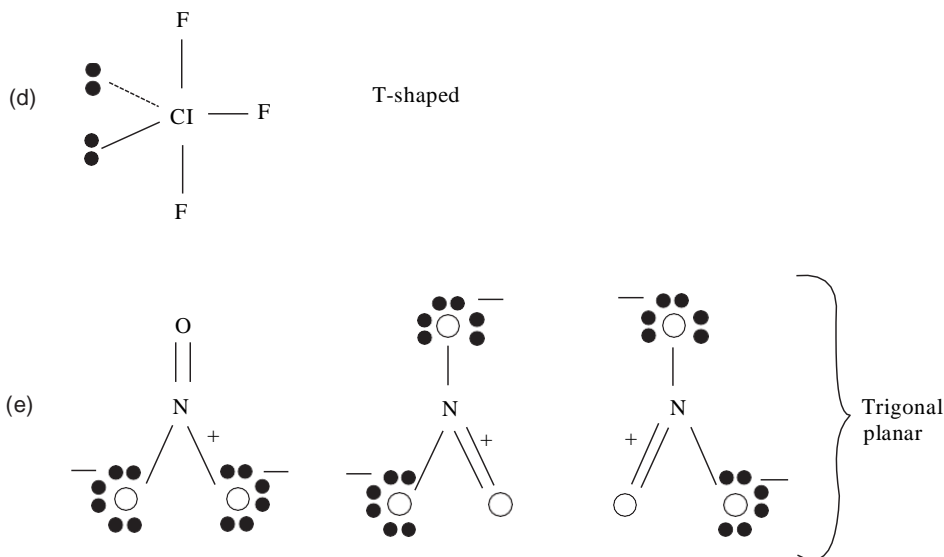
Numerous non-metallic essential particles (H_2 , Cl_2 , F_2 and so forth.) and in addition atoms containing different molecules, for example, CH_4 , HNO_3 , H_2O and HF are covalently fortified. Moreover, this kind of holding is found in basic solids, for example, precious stone (carbon), silicon, and germanium and other strong mixes made out of components that are situated on the right-hand side of the occasional table, for example, gallium arsenide (GaAs), indium antimonide (InSb), and silicon carbide (SiC).

Example: Draw Lewis structures for the following molecules, including all formal charges. Also indicate the geometry of each central atom in the molecule. Include resonance structures where appropriate.

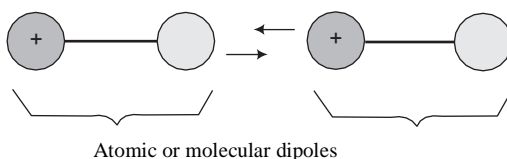
- (a) BeI_2
- (b) HCl
- (c) IF_2
- (d) ClF_3
- (e) NO_3

Solution:





Metallic Bonds: Metallic bonding, the last essential bonding sort, is found in metals and their alloys. A moderately basic model has been recommended that practically approximates the bonding plan. Metallic materials have one, two, or at most, three valence electrons. With this model, these valence electrons are not bound to a specific molecule in particular and are pretty much allowed to float all through the whole metal. They might be considered having a place with the metal overall, or framing an “ocean of electrons” or an “electron cloud.” The rest of the non-valence electrons and nuclear cores shape called ions core, have a net positive charge rise to in size to the aggregate valence electron charge per iota. Figure 2.10 is a schematic outline of metallic holding. The free electrons shield the decidedly charged particle centres from commonly horrible electrostatic strengths, which they would some way or another apply upon each other; consequently, the metallic bond is non-directional in character. Likewise, these free electrons go about as a “paste” to hold the particle cores together. Metallic bonding is found in the occasional table for Group IA and IIA elements and, truth be told, for every elemental metal. Some broad conduct of the different material sorts (i.e., metals, earthenware production, polymers) might be clarified by holding sort. For instance, metals are great channels of both power and warmth, as a result of their free electrons. By the method for difference, ionically and covalently reinforced materials are regularly electrical and warm separators, because of the nonappearance of vast quantities of free electrons.



Schematic illustration of van der Waals bonding between two dipoles.

quick and brief mutilations of this electrical symmetry for a portion of the iotas or atoms, and the formation of little electric dipoles, as shown in Figure 2.12b. One of these dipoles can thus deliver a relocation of the electron conveyance of an adjoining particle or atom, which instigates the second one likewise to wind up a dipole that is then pitifully pulled in or attached to the main; this is one sort of van der Waals bonding. These alluring powers may exist between huge quantities of particles or atoms, which strengths are impermanent and vacillate with time.

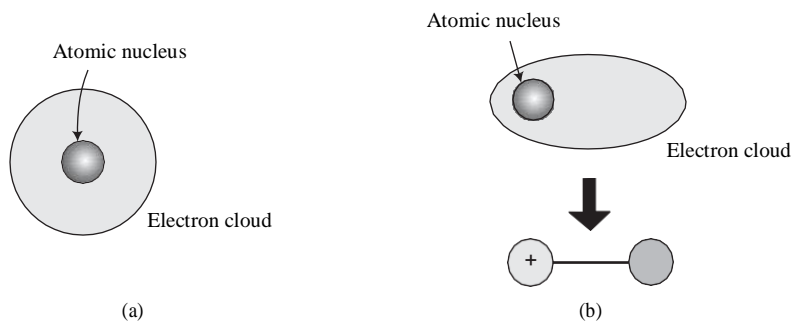


Figure: Schematic representations of (a) an electrically symmetric atom and (b) an induced atomic dipole.

Since the electrons might be on one side of the molecule or the other, a dipole is framed: the + nucleus at the centre, and the electron outside. Since the electron moves, the dipole vacillates. This vacillation in particle A produces a fluctuating electric field that is felt by the electrons of a nearby iota, B. Molecule B then spellbinds so that its external electrons are in favour of the atom nearest to the + side (or inverse to the – side) of the dipole in A.

Polar Molecule-induced Dipole Bonds: Perpetual dipole minutes exist in a few atoms by temperance of an unbalanced course of action of emphatically and contrarily charged districts; such particles are named polar particles. Figure 2.13 is a schematic representation of a hydrogen chloride atom; a changeless dipole minute emerges from net positive and negative charges that are individually connected with the hydrogen and chlorine finishes of the HCl molecule. Polar atoms can likewise instigate dipoles in contiguous nonpolar particles, and a bond will shape as a consequence of alluring powers between the two

atoms. Besides, the extent of this bond will be more noteworthy than for fluctuating prompted dipoles.

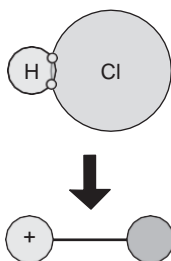


Figure: Schematic representation of a polar hydrogen chloride (HCl) molecule.

We can summarise this: It is another sort of optional bond which exists with asymmetric particles, additionally called polar atoms on account of positive and negative charged locales. A lasting dipole minute emerges from net positive and negative charges that are separately connected with the hydrogen and chlorine finishes of the HCl particle, prompting to holding. The size of this bond will be more noteworthy than for fluctuating instigated dipoles. These two sorts of bonds are likewise called van der Waals bonds. Third sort of auxiliary bond is the hydrogen bond. It is sorted independently in light of the fact that it creates the most grounded strengths of fascination in this class.

Permanent Dipole Bonds: Van der Waals forces will likewise exist between contiguous polar particles. The related holding energies are essentially more noteworthy than for bonds including initiated dipoles. The most grounded auxiliary holding sort, the hydrogen bond, is an exceptional instance of polar particle holding. It happens between atoms in which hydrogen is covalently bonded to fluorine (as in HF), oxygen (as in H_2O), and nitrogen (as in HNO_3). For every H—F, H—O, or H—N bond, the single hydrogen electron is imparted to the next particle. Along these lines, the hydrogen end of the bond is basically an emphatically charged uncovered proton that is unshielded by any electrons. This very decidedly charged end of the particle is fit for a solid appealing power with the negative end of a neighbouring atom, as exhibited in Figure

for HF. Generally, this single proton structures a scaffold between two contrarily charged atoms. The greatness of the hydrogen bond is by and large more noteworthy than that of alternate sorts of optional bonds and might be as high as 51 kJ/mol (0.52 eV/ particle), as appeared in melting and bubbling temperatures for hydrogen fluoride and water are strangely high in light of their low subatomic weights, as an outcome of hydrogen bonding.

Secondary Bonding or van der Waals Bonding

Both van der Waals and hydrogen bonds are named auxiliary, being powerless in contrast with the essential ones. They result from appealing strengths between electric dipoles, of which there are two sorts—instigated and changeless. For the hydrogen bond, very polar atoms frame when hydrogen covalently bonds to a non-metallic component, for example, fluorine.

Assignment

1. (a) Differentiate between atomic mass and atomic weight.
(b) In one amu of a material contains how many grams?
2. Give the electron configurations for the following ions: P^{5+} , P^{3-} , Sn^{4+} and Se^{2-} .
3. To what group in the periodic table would an element with atomic number 112 belong?
4. (a) What electron sub-shell is being filled for the rare earth series of elements on the periodic table?
(b) What electron sub-shell is being filled for the actinide series?
5. (a) Briefly cite the main differences between ionic, covalent, and metallic bonding.
(b) State the Pauli exclusion principle.
6. What type(s) of bonding would be expected for each of the following materials: solid xenon, calcium fluoride, bronze, cadmium telluride, rubber, and tungsten?
7. Explain why hydrogen fluoride (HF) has a higher boiling temperature than hydrogen chloride (HCl) even though HF has a lower molecular weight?

Geometry of Lattices

In this Chapter the general static properties of crystals, as well as possibilities to observe crystal structures, are reviewed. We emphasize basic principles of the crystal structure description. More detailed information can be obtained, e.g., from the books [1, 4, 5].

Periodicity: Crystal Structures

Most of solid materials possess crystalline structure that means spatial periodicity or translation symmetry. All the lattice can be obtained by repetition of a building block called basis. We assume that there are 3 non-coplanar vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 that leave all the properties of the crystal unchanged after the shift as a whole by any of those vectors. As a result, any lattice point \mathbf{R}^J could be obtained from another point \mathbf{R} as

$$\mathbf{R}^J = \mathbf{R} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3 \quad (1.1)$$

where m_i are integers. Such a lattice of building blocks is called the Bravais lattice. The crystal structure could be understood by the combination of the properties of the building block (basis) and of the Bravais lattice. Note that

- There is no unique way to choose \mathbf{a}_i . We choose \mathbf{a}_1 as shortest period of the lattice, \mathbf{a}_2 as the shortest period not parallel to \mathbf{a}_1 , \mathbf{a}_3 as the shortest period not coplanar to \mathbf{a}_1 and \mathbf{a}_2 .
- Vectors \mathbf{a}_i chosen in such a way are called primitive.
- The volume cell enclosed by the primitive vectors is called the primitive unit cell.
- The volume of the primitive cell is V_0

$$V_0 = (\mathbf{a}_1[\mathbf{a}_2\mathbf{a}_3]) \quad (1.2)$$

The natural way to describe a crystal structure is a set of point group operations which involve operations applied around a point of the lattice. We shall see that symmetry provide important restrictions upon vibration and electron properties (in particular, spectrum degeneracy). Usually are discussed:

Rotation, C_n : Rotation by an angle $2\pi/n$ about the specified axis. There are restrictions for n . Indeed, if a is the lattice constant, the quantity $b = a + 2a \cos \phi$ (see Fig.) Consequently, $\cos \phi = i/2$ WHERE i is integer.

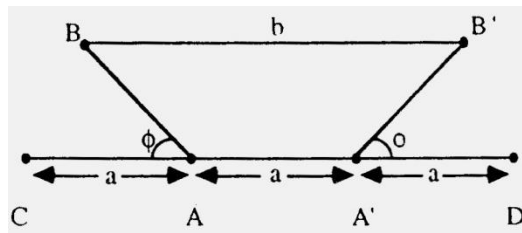


Figure: On the determination of rotation symmetry

Inversion, I : Transformation $\mathbf{r} \rightarrow -\mathbf{r}$, fixed point is selected as origin (lack of inversion symmetry may lead to piezoelectricity);

Reflection, σ : Reflection across a plane;

Improper Rotation, S_n : Rotation C_n , followed by reflection in the plane normal to the rotation axis.

Examples

Now we discuss few examples of the lattices.

One-Dimensional Lattices - Chains

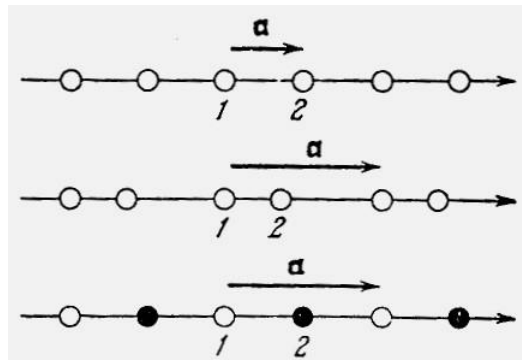


Figure: One dimensional lattices

1D chains are shown in Fig. We have only 1 translation vector $|\mathbf{a}_1| = a$, $V_0 = a$.

PERIODICITY: CRYSTAL STRUCTURES

White and black circles are the atoms of different kind. A is a primitive lattice with one atom in a primitive cell; b and c are composite lattice with two atoms in a cell.

Two-Dimensional Lattices

There are 5 basic classes of 2D lattices (see Fig.)

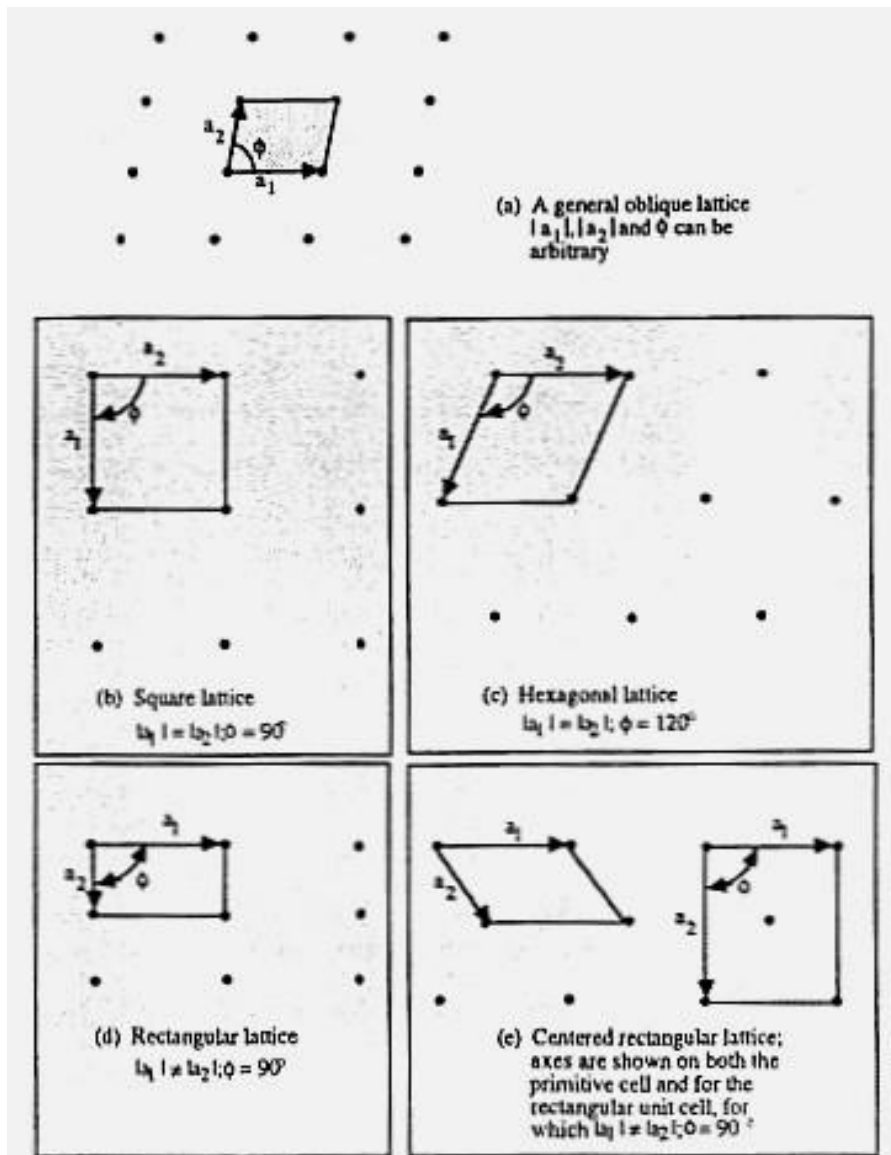


Figure: The five classes of 2D lattices (from the book [4]).

Three-Dimensional Lattices

There are 14 types of lattices in 3 dimensions. Several primitive cells is shown in Fig. The types of lattices differ by the relations between the lengths a_i and the angles α_i .

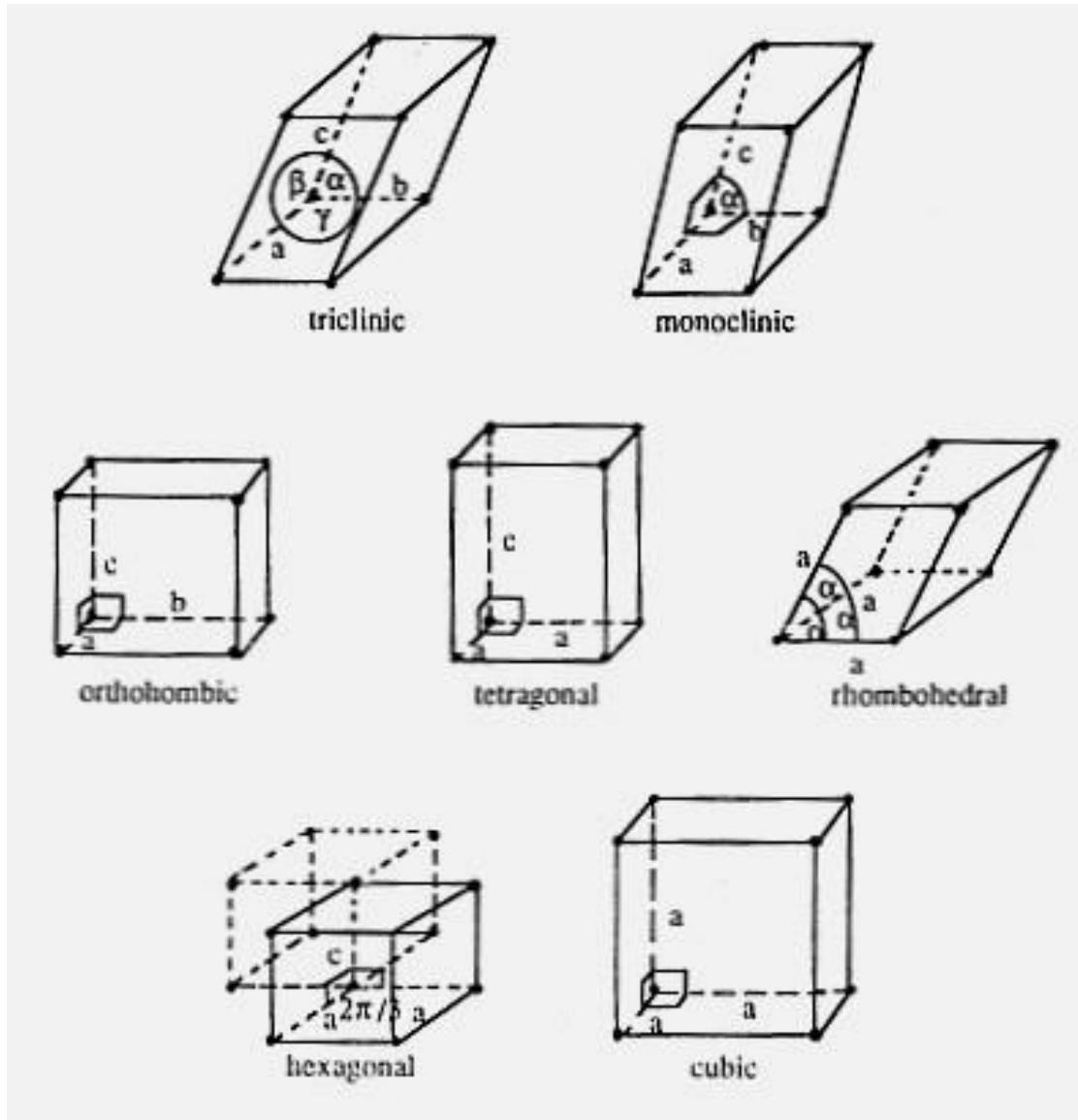


Figure: Types of 3D lattices

We will concentrate on cubic lattices which are very important for many materials.

Cubic and Hexagonal Lattices. Some primitive lattices are shown in Fig. 1.5. a, b, and c show cubic lattices. a is the simple cubic lattice (1 atom per primitive cell), b is the body centered cubic lattice ($1/8 \times 8 + 1 = 2$ atoms), c is face-centered lattice ($1/8 \times 8 + 1/2 \times 6 = 4$ atoms). The part c of the Fig. shows hexagonal cell.

PERIODICITY: CRYSTAL STRUCTURES

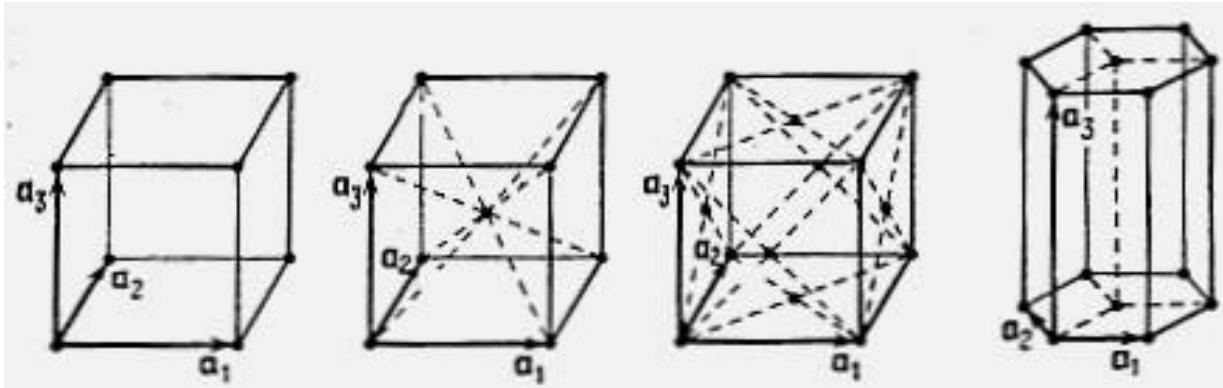


Figure: Primitive lattices

We shall see

that discrimination between simple and complex lattices is important, say, in analysis of lattice vibrations.

The Wigner-Seitz cell

As we have mentioned, the procedure of choose of the elementary cell is not unique and sometimes an arbitrary cell does not reflect the symmetry of the lattice (see, e. g., Fig. 1.6, and 1.7 where specific choices for cubic lattices are shown). There is a very convenient

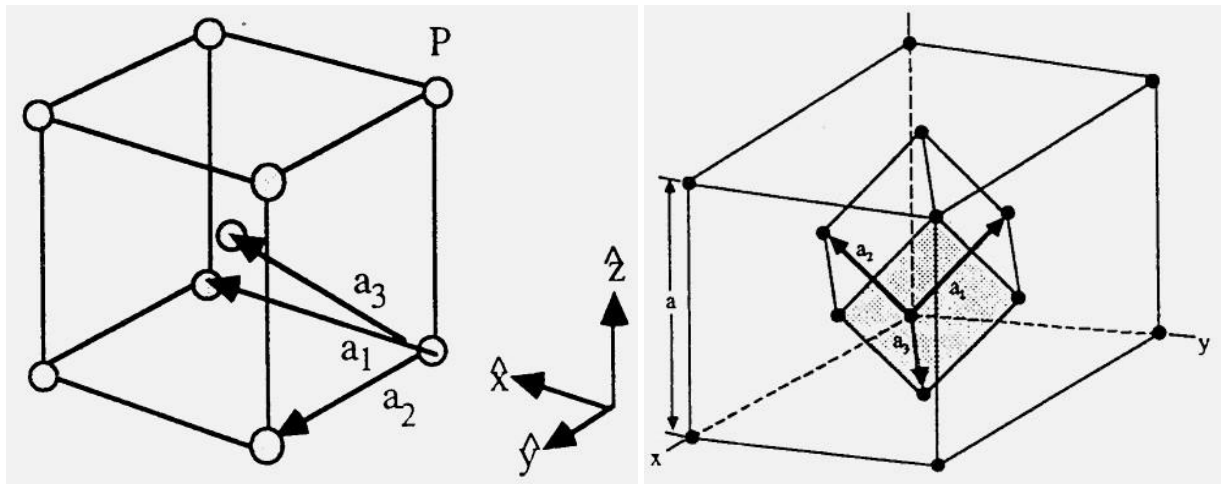


Figure: Primitive vectors for bcc (left panel) and (right panel) lattices.

procedure to choose the cell which reflects the symmetry of the lattice. The procedure is as follows:

1. Draw lines connecting a given lattice point to all neighboring points.
2. Draw bisecting lines (or planes) to the previous lines.

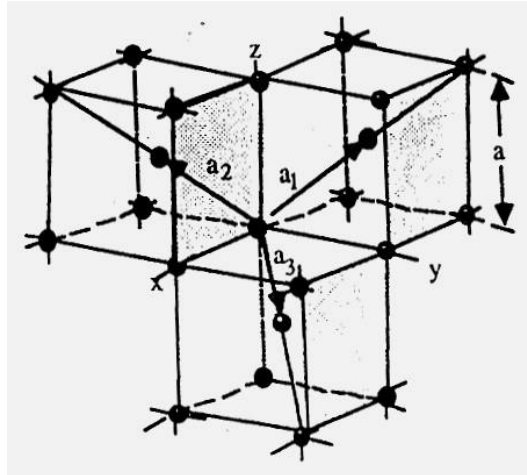


Figure: More symmetric choice of lattice vectors for bcc lattice.

The procedure is outlined in Fig. For complex lattices such a procedure should be done for one of simple sublattices. We shall come back to this procedure later analyzing electron band structure.

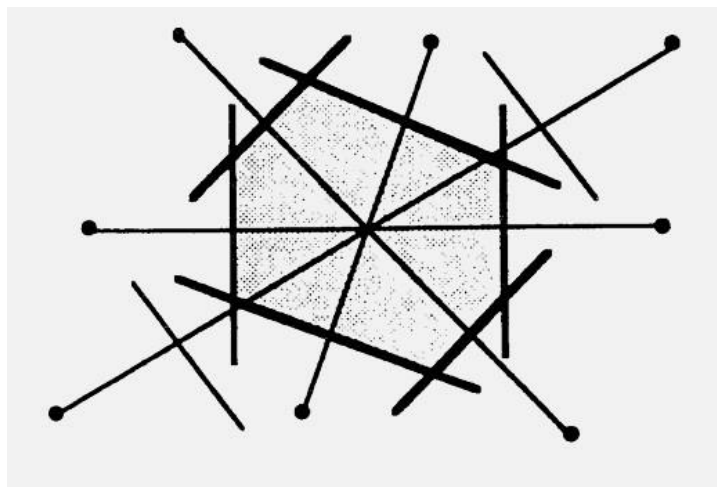


Figure: To the determination of Wigner-Seitz cell.

Temperature Coefficient of Resistance

You might have noticed on the table for specific resistances that all figures were specified at a temperature of 20° Celsius. If you suspected that this meant specific resistance of a material may change with temperature, you were right! Resistance values for conductors at any temperature other than the standard temperature (usually specified at 20 Celsius) on the specific resistance table must be determined through yet another formula:

$$R = R_{\text{ref}} [1 + \alpha(T - T_{\text{ref}})]$$

Where,

R = Conductor resistance at temperature “T”

R_{ref} = Conductor resistance at reference temperature
T_{ref}, usually 20°C, but sometimes 0°C.

α = Temperature coefficient of resistance for
conductor material.

T = Conductor temperature in degrees Celsius.

T_{ref} = Reference temperature that α is specified at
for the conductor material

The “alpha” (α) constant is known as the temperature coefficient of resistance and symbolizes the resistance change factor per degree of temperature change. Just as all materials have a certain specific resistance (at 20° C), they also change resistance according to temperature by certain amounts. For pure metals, this coefficient is a positive number, meaning that resistance increases with increasing temperature. For the elements carbon, silicon, and germanium, this coefficient is a negative number, meaning that resistance decreases with increasing temperature. For some metal alloys, the temperature coefficient of resistance is very close to zero, meaning that the resistance hardly changes at all with variations in temperature (a good property if you want to build a precision resistor out of metal wire!). The following table gives the temperature coefficients of resistance for several common metals, both pure and alloy

Temperature Coefficients of Resistance at 20 Degrees Celsius

Material	Element/Alloy	“alpha” per degree Celsius
Nickel	Element	0.005866
Iron	Element	0.005671
Molybdenum	Element	0.004579
Tungsten	Element	0.004403
Aluminum	Element	0.004308
Copper	Element	0.004041
Silver	Element	0.003819
Platinum	Element	0.003729
Gold	Element	0.003715
Zinc	Element	0.003847
Steel*	Alloy	0.003
Nichrome	Alloy	0.00017
Nichrome V	Alloy	0.00013
Manganin	Alloy	+/- 0.000015

- Most conductive materials change specific resistance with changes in temperature. This is why figures of specific resistance are always specified at a standard temperature (usually 20° or 25° Celsius).
- The resistance-change factor per degree Celsius of temperature change is called the temperature coefficient of resistance. This factor is represented by the Greek lower-case letter “alpha” (α).
- A positive coefficient for a material means that its resistance increases with an increase in temperature. Pure metals typically have positive temperature coefficients of resistance. Coefficients approaching zero can be obtained by alloying certain metals.

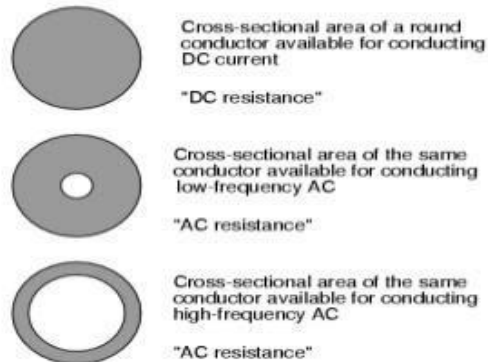
Skin Effect

The non-uniform distribution of electric current over the surface or skin of the conductor carrying AC is called the skin effect. In other words, the concentration of charge is more near the surface as compared to the core of the conductor. The ohmic resistance of the conductor is increased due to the concentration of current on the surface of the conductor.

Skin effect increases with the increase in frequency. At low frequency, such as 50Hz, there is a small increase in the current density near the surface of the conductor; but, at high frequencies, such as radio frequency, practically the whole of the currents flows on the surface of the conductor. If DC current (frequency=0) is passed in a conductor, the current is uniformly distributed over the cross-section of the conductors.

Skin Effect

- ❑ At 60 Hz in copper, the skin depth is about 0.65 μm .
- ❑ Due to the skin effect AC resistance increases in conductor
- ❑ At high frequencies the skin depth becomes much smaller.



$$R_{AC} = (R_{DC})(k) \sqrt{f}$$

Where,

R_{AC} = AC resistance at given frequency "f"

R_{DC} = Resistance at zero frequency (DC)

k = Wire gauge factor (see table below)

f = Frequency of AC in MHz (megahertz)

Why skin effect occurs?

Let us consider the conductor is made up of a number of concentric cylinders. When AC is passed in a conductor, the magnetic flux induces in it. The magnetic flux linking a cylindrical element near the center is greater than that linking another cylindrical element near the surface of the conductor. This is due to the fact

that the center cylindrical element is surrounded by both the internal as well as the external flux, while the external cylindrical element is surrounded by the external flux only. The self-inductance in the inner cylindrical element is more and, therefore, will offer a greater inductive reactance than the outer cylindrical element. This difference in the inductive reactance gives a tendency to the current to concentrate towards the surface or skin of the conductor.

The current density is maximum at the surface of the conductor and minimum at the center of the conductor. The effect is equivalent to a reduction of the cross-section area of the conductor and, therefore the effective resistance of the conductor is increased.

Factors affecting skin effect

1. **Frequency** – Skin effect increases with the increase in frequency.
2. **Diameter** – It increases with the increase in diameter of the conductor.
3. **The shape of the conductor** – Skin effect is more in the solid conductor and less in the stranded conductor because the surface area of the solid conductor is more.
4. **Type of material** – Skin effect increase with the increase in the permeability of the material (Permeability is the ability of material to support the formation of the magnetic field).

Points-to-remember

1. The Skin effect is negligible if the frequency is less than the 50Hz and the diameter of the conductor is less than the 1cm.
2. In the stranded conductors like ACSR (Aluminium Conductor Steel Reinforced) the current flows mostly in the outer layer made of aluminum, while the steel near the center carries no current and gives high tensile strength to the conductor. The concentration of current near the surface enabled the use of ACSR conductor.

Hall Effect

If an electric current flows through a conductor in a magnetic field, the magnetic field exerts a transverse force on the moving charge carriers which tends to push them to one side of the conductor. This is most evident in a thin flat conductor as illustrated. A buildup of charge at the sides of the conductors will balance this magnetic influence, producing a measurable voltage between the two sides of the conductor. The presence of this measurable transverse voltage is called the Hall effect after E. H. Hall who discovered it in 1879. Note that the direction of the current I in the diagram is that of conventional current, so that the motion of electrons is in the opposite direction. That further confuses all the **Right-Hand Rule** manipulations you have to go through to get the direction of the forces.

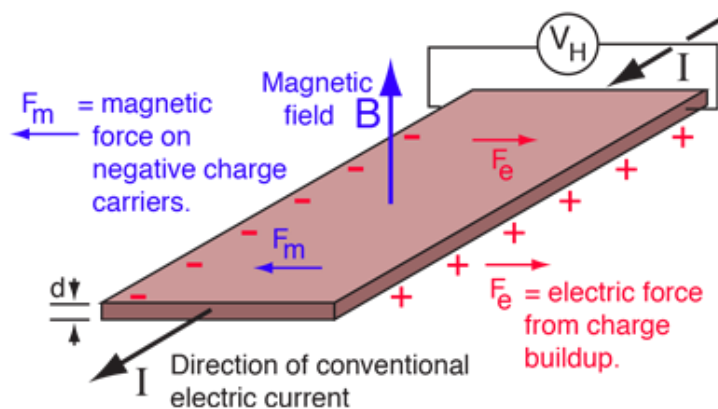
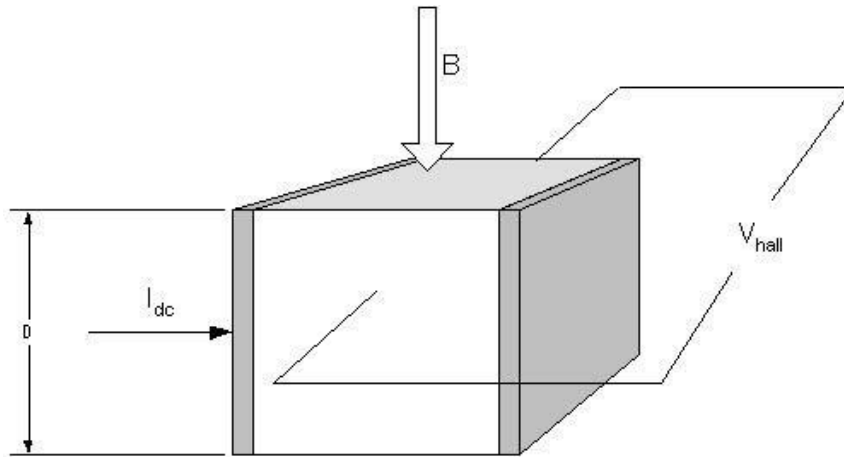


Figure: Hall probe for magnetic field measurement



B = magnetic field

I_{dc} = bias current

D = thickness of Hall sensor

R_h = material constant (Hall Constant)

$$V_{hall} = \frac{R_h \cdot I_{dc} \cdot B}{D}$$