AE8007 / Aircraft Materials

UNIT-1- *ELEMENTS OF AEROSPACE MATERIALS*

Structure of solid materials – Atomic structure of materials – crystal structure – miller indices – density – packing factor – space lattices – x-ray diffraction – imperfection in crystals – physical metallurgy - general requirements of materials for aerospace applications

Importance of Materials

A material is defined as a substance (most often a solid, but other condensed phases can be included) that is intended to be used for certain applications. There are a myriad of materials around us—they can be found in anything from buildings to spacecrafts. Materials can generally be divided into two classes: crystalline and non-crystalline. The traditional examples of materials are metals, ceramics and polymers. New and advanced materials that are being developed include semiconductors, nanomaterials, biomaterials etc.

The material of choice of a given era is often a defining point. Phrases such as Stone Age, Bronze Age, Iron Age, and Steel Age are great examples. Originally deriving from the manufacture of ceramics and its putative derivative metallurgy, materials science is one of the oldest forms of engineering and applied science. Modern materials science evolved directly from metallurgy, which itself evolved from mining and (likely) ceramics and the use of fire. A major breakthrough in the understanding of materials occurred in the late 19th century, when the American scientist Josiah Willard Gibbs demonstrated that the thermodynamic properties related to atomic structure in various phases are related to the physical properties of a material. Important elements of modern materials science are a product of the space race: the understanding and engineering of the metallic alloys, and silica and carbon materials, used in the construction of space vehicles enabling the exploration of space. Materials science has driven, and been driven by, the development of revolutionary technologies such as plastics, semiconductors, and biomaterials.

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Before the 1960s (and in some cases decades after), many materials science departments were named metallurgy departments, reflecting the 19th and early 20th century emphasis on metals. The field has since broadened to include every class of materials, including ceramics, polymers, semiconductors, magnetic materials, medical implant materials, biological materials and nanomaterials (materiomics).

Historical Perspective

Materials are so important in the development of civilization that we associate ages with them. In the origin of human life on earth, the Stone Age, people used only natural materials like stone, clay, skins, and wood. When people found copper and how to make it harder by alloying, the bronze Age started about 3000 BC. The use of iron and steel, stronger materials that gave advantage in wars started at about 1200 BC. The next big step was the discovery of a cheap process to make steel around 1850, which enabled the railroads and the building of the modern infrastructure of the industrial world.

Classification of Materials

Like many other things, materials are classified in groups, so that our brain can handle the complexity. One could classify them according to structure, or properties, or use. The one that we will use is according to the way the atoms are bound together:

Metals: The valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the ions together. Metals are usually strong, conduct electricity and heat well and are opaque to light (shiny if polished). Examples: aluminum, steel, brass, gold.

Semiconductors: The bonding is covalent (electrons are shared between atoms). Their electrical properties depend extremely strongly on minute proportions of contaminants. They are opaque to visible light but transparent to the infrared. Examples: Si, Ge, GaAs.

Ceramics: Atoms behave mostly like either positive or negative ions, and are bound by Coulomb forces between them. They are usually combinations of metals

or semiconductors with oxygen, nitrogen or carbon (oxides, nitrides, and carbides).Examples: glass, porcelain, many minerals.

Polymers: are bound by covalent forces and also by weak van der Waals forces, and usually based on H, C and other non-metallic elements. They decompose at moderate temperatures (100 – 400 C), and are lightweight. Other properties vary greatly. Examples: plastics (nylon, teflon, polyester) and rubber. Other categories are not based on bonding. A particular microstructure identifies

Composites: Composites made of different materials in intimate contact (example: fiberglass, concrete, wood) to achieve specific properties. **Biomaterials** can be any type of material that is biocompatible and used, for instance, to replace human body parts.

Advanced Materials

Materials used in "High-Tec" applications, usually designed for maximum performance, and normally expensive. Examples are titanium alloys for supersonic airplanes, magnetic alloys for computer disks, special ceramics for the heat shield of the space shuttle, etc.

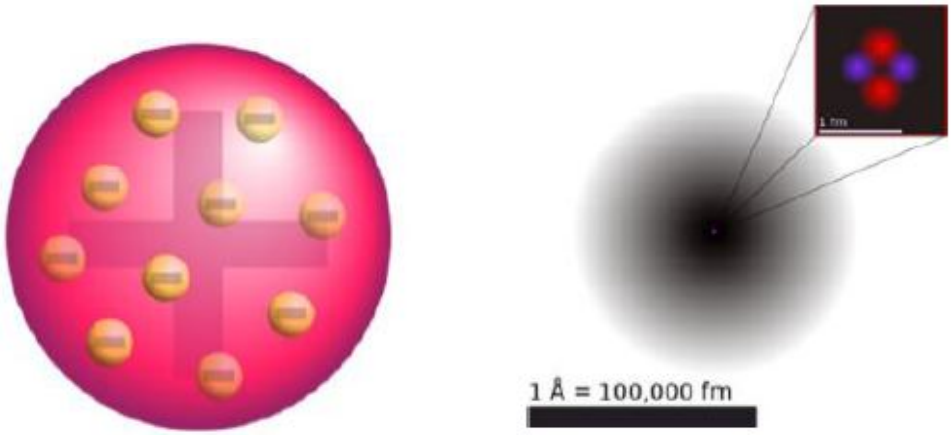
Modern Material's Needs

- Engine efficiency increases at high temperatures: requires high temperature withstanding 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.

Atomic models

Thomson atomic model

A schematic presentation of the plum pudding model of the atom; in Thomson's mathematical model the "corpuscles" (or modern electrons) were arranged non-randomly, in rotating rings



The current model of the sub-atomic structure involves a dense nucleus surrounded by a probabilistic "cloud" of electrons

The **plum pudding model** was a model of the atom that incorporated the recently discovered electron, and was proposed by J. J. Thomson in 1904. Thomson had discovered the electron in

1897. The plum pudding model was abandoned after discovery of the atomic nucleus. The plum pudding model of the atom is also known as the "Blueberry Muffin" model.

In this model, the atom is composed of electrons (which Thomson still called "corpuscles", though G. J. Stoney had proposed that atoms of electricity be called electrons in 1894) surrounded by a soup of positive charge to balance the electrons' negative charges, like negatively charged "raisins" surrounded by positively charged "pudding". The electrons (as we know them today) were thought to be positioned throughout the atom, but with many structures possible for positioning multiple electrons, particularly rotating rings of electrons (see below). Instead of a soup, the atom was also sometimes said to have had a "cloud" of positive charge.

With this model, Thomson abandoned his earlier "nebular atom" hypothesis in which the atom was composed of immaterial vortices. Now, at least part of the atom was to be composed of Thomson's particulate negative "corpuscles", although the rest of the positively charged part of the atom remained somewhat nebulous and ill-defined.

The 1904 Thomson model was disproved by the 1909 gold foil experiment of Hans Geiger and Ernest Marsden. This was interpreted by Ernest Rutherford in 1911 to imply a very small nucleus of the atom containing a very high positive charge (in the case of gold, enough to balance about 100 electrons), thus leading to the Rutherford model of the atom. Although gold has an atomic number of 79, immediately after Rutherford's paper appeared in 1911 Antonius Van den Broek made the intuitive suggestion that atomic number is nuclear charge. The matter required experiment to decide. Henry Moseley's work showed experimentally in 1913 (see Moseley's law) that the effective nuclear charge was very close to the atomic number (Moseley found only one unit difference), and Moseley referenced only the papers of Van den Broek and Rutherford. This work culminated in the solar-system-like (but quantum-limited) Bohr model of the atom in the same year, in which a nucleus containing an atomic number of positive charge is surrounded by an equal number of electrons in orbital shells. Bohr had also inspired Moseley's work.

Thomson's model was compared (though not by Thomson) to a British dessert called plum pudding, hence the name. Thomson's paper was published in the March 1904 edition of the Philosophical Magazine, the leading British science journal of the day. In Thomson's view: the atoms of the elements consist of a number of negatively electrified corpuscles enclosed in a sphere of uniform positive electrification.

In this model, the electrons were free to rotate within the blob or cloud of positive substance.

These orbits were stabilized in the model by the fact that when an electron moved farther from the center of the positive cloud, it felt a larger net positive inward force, because there was more material of opposite charge, inside its orbit (see Gauss's law). In Thomson's model, electrons were free to rotate in rings which

were further stabilized by interactions between the electrons, and spectra were to be accounted for by energy differences of different ring orbits. Thomson attempted to make his model account for some of the major spectral lines known for some elements, but was not notably successful at this. Still, Thomson's model (along with a similar Saturnian ring model for atomic electrons, also put forward in 1904 by Nagaoka after James Clerk Maxwell's model of Saturn's rings), were earlier harbingers of the later and more successful solar-system-like Bohr model of the atom.

Rutherford model

Rutherford overturned Thomson's model in 1911 with his well-known gold foil experiment in which he demonstrated that the atom has a tiny, heavy nucleus. Rutherford designed an experiment to use the alpha particles emitted by a radioactive element as probes to the unseen world of atomic structure.

Rutherford presented his own physical model for subatomic structure, as an interpretation for the unexpected experimental results. In it, the atom is made up of a central charge (this is the modern atomic nucleus, though Rutherford did not use the term "nucleus" in his paper) surrounded by a cloud of (presumably) orbiting electrons. In this May 1911 paper, Rutherford only commits himself to a small central region of very high positive or negative charge in the atom.

For concreteness, consider the passage of a high speed α particle through an atom having a positive central charge N e, and surrounded by a compensating charge of N electrons.

From purely energetic considerations of how far particles of known speed would be able to penetrate toward a central charge of 100 e, Rutherford was able to calculate that the radius of his gold central charge would need to be less (how much less could not be told) than 3.4×10^{-14} metres. This was in a gold atom known to be 10−10 meters or so in radius—a very surprising finding, as it implied a strong central charge less than 1/3000th of the diameter of the atom.

The Rutherford model served to concentrate a great deal of the atom's charge and mass to a very small core, but didn't attribute any structure to the remaining electrons and remaining atomic mass. It did mention the atomic model of Hantaro

Nagaoka, in which the electrons are arranged in one or more rings, with the specific metaphorical structure of the stable rings of Saturn. The plum pudding model of J.J. Thomson also had rings of orbiting electrons. Jean Baptiste Perrin claimed in his Nobel Lecture that he was the first one to suggest the model in his paper dated1901.

The Rutherford paper suggested that the central charge of an atom might be "proportional" to its atomic mass in hydrogen mass units u (roughly 1/2 of it, in Rutherford's model). For gold, this mass number is 197 (not then known to great accuracy) and was therefore modeled by Rutherford to be possibly 196 u. However, Rutherford did not attempt to make the direct connection of central charge to atomic number, since gold's "atomic number" (at that time merely its place number in the periodic table) was 79, and Rutherford had modeled the charge to be about + 100 units (he had actually suggested 98 units of positive charge, to make half of 196). Thus, Rutherford did not formally suggest the two numbers (periodic table place, 79, and nuclear charge, 98 or 100) might be exactly the same.

Bohr model

In the early 20th century, experiments by Ernest Rutherford established that atoms consisted of a diffuse cloud of negatively charged electrons surrounding a small, dense, positively charged nucleus. Given this experimental data, Rutherford naturally considered a planetary-model atom, the Rutherford model of 1911 – electrons orbiting a solar nucleus – however, said planetarymodel atom has a technical difficulty. The laws of classical mechanics (i.e. the Larmor formula), predict that the electron will release electromagnetic radiation while orbiting a nucleus. Because the electron would lose energy, it would rapidly spiral inwards, collapsing into the nucleus on a timescale of around 16 picoseconds. This atom model is disastrous, because it predicts that all atoms are unstable.

Also, as the electron spirals inward, the emission would rapidly increase in frequency as the orbit got smaller and faster. This would produce a continuous smear, in frequency, of electromagnetic radiation. However, late 19th century experiments with electric discharges have shown that atoms will only emit light (that is, electromagnetic radiation) at certain discrete frequencies.

To overcome this difficulty, Niels Bohr proposed, in 1913, what is now called the Bohr model of the atom. He suggested that electrons could only have certain classical motions:

1. Electrons in atoms orbit the nucleus.
2. The electrons can only orbit stably, without radiating, in certain orbits (called by Bohr the "stationary orbits") at a certain discrete set of distances from the nucleus. These orbits are associated with definite energies and are also called energy shells or energy levels. In these orbits, the electron's acceleration does not result in radiation and energy loss as required by classical electromagnetics.
3. Electrons can only gain and lose energy by jumping from one allowed orbit to another, absorbing or emitting electromagnetic radiation with a frequency ν determined by the energy difference of the levels according to the Planck relation

Where h is Planck's constant. The frequency of the radiation emitted at an orbit of period T is as it would be in classical mechanics; it is the reciprocal of the classical orbit period:
The significance of the Bohr model is that the laws of classical mechanics apply to the motion of the electron about the nucleus only when restricted by a quantum rule. Although rule 3 is not completely well defined for small orbits, because the emission process involves two orbits with two different periods, Bohr could determine the energy spacing between levels using rule 3 and come to an exactly correct quantum rule: the angular momentum L is restricted to be an integer multiple of a fixed unit:

$$L = n\frac{h}{2\pi} = n\hbar$$

where n = 1, 2, 3, ... is called the principal quantum number, and ħ = h/2π. The lowest value of n is 1; this gives a smallest possible orbital radius of 0.0529 nm known as the Bohr radius. Once an electron is in this lowest orbit, it can get no closer to the proton. Starting from the angular momentum quantum rule, Bohr was able to calculate the energies of the allowed orbits of the hydrogen atom and other hydrogen-like atoms and ions. Other points are:

1. Like Einstein's theory of the Photoelectric effect, Bohr's formula assumes that during a quantum jump a discrete amount of energy is radiated. However, unlike Einstein, Bohr stuck to the classical Maxwell theory of the

electromagnetic field. Quantization of the electromagnetic field was explained by the discreteness of the atomic energy levels; Bohr did not believe in the existence of photons.

2. According to the Maxwell theory the frequency ν of classical radiation is equal to the rotation frequency νrot of the electron in its orbit, with harmonics at integer multiples of this frequency. This result is obtained from the Bohr model for jumps between energy levels En and En−k when k is much smaller than n. These jumps reproduce the frequency of the k-th harmonic of orbit n. For sufficiently large values of n (so-called Rydberg states), the two orbits involved in the emission process have nearly the same rotation frequency, so that the classical orbital frequency is not ambiguous. But for small n (or large k), the radiation frequency has no unambiguous classical interpretation. This marks the birth of the correspondence principle, requiring quantum theory to agree with the classical theory only in the limit of large quantum numbers.
3. The Bohr-Kramers-Slater theory (BKS theory) is a failed attempt to extend the Bohr model which violates the conservation of energy and momentum in quantum jumps, with the conservation laws only holding on average. Bohr's condition, that the angular momentum is an integer multiple of $\hbar$ was later reinterpreted in 1924 by de Broglie as a standing wave condition: the electron is described by a wave and a whole number of wavelengths must fit along the circumference of the electron's orbit

$$n\lambda = 2\pi r.$$

Substituting de Broglie's wavelength of h/p reproduces Bohr's rule. In 1913, however, Bohr justified his rule by appealing to the correspondence principle, without providing any sort of wave interpretation. In 1913, the wave behavior of matter particles such as the electron (i.e., matter waves) was not suspected.:

Atomic bonding in solids

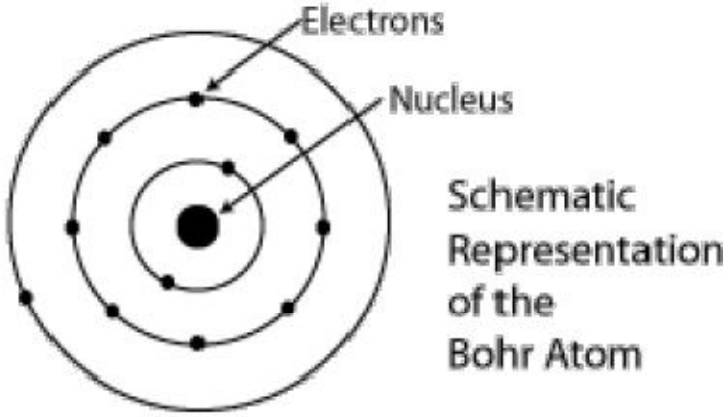
From elementary chemistry it is known that the atomic structure of any element is made up of a positively charged nucleus surrounded by electrons revolving around it. An element’s atomic number indicates the number of positively charged protons in the nucleus.

The atomic weight of an atom indicates how many protons and neutrons in the nucleus. To determine the number of neutrons in an atom, the atomic number is simply subtracted from the atomic weight.

Atoms like to have a balanced electrical charge. Therefore, they usually have negatively charged electrons surrounding the nucleus in numbers equal to the

number of protons. It is also known that electrons are present with different energies and it is convenient to consider these electrons surrounding the nucleus in energy "shells." For example, magnesium, with an atomic number of 12, has two electrons in the inner shell, eight in the second shell and two in the outer shell.

All chemical bonds involve electrons. Atoms will stay close together if they have a shared interest in one or more electrons. Atoms are at their most stable when they have no partially filled electron shells. If an atom has only a few electrons in a shell, it will tend to lose them to empty the shell. These elements are metals. When metal atoms bond, a metallic bond occurs.
When an atom has a nearly full electron shell, it will try to find electrons from another atom so that it can fill its outer shell. These elements are usually described as nonmetals. The bond between two nonmetal atoms is usually a covalent bond. Where metal and nonmetal atom come together an ionic bond occurs. There are also other, less common, types of bond but the details are beyond the scope of this material. On the next few pages, the Metallic, Covalent and Ionic bonds will be covered in more detail.



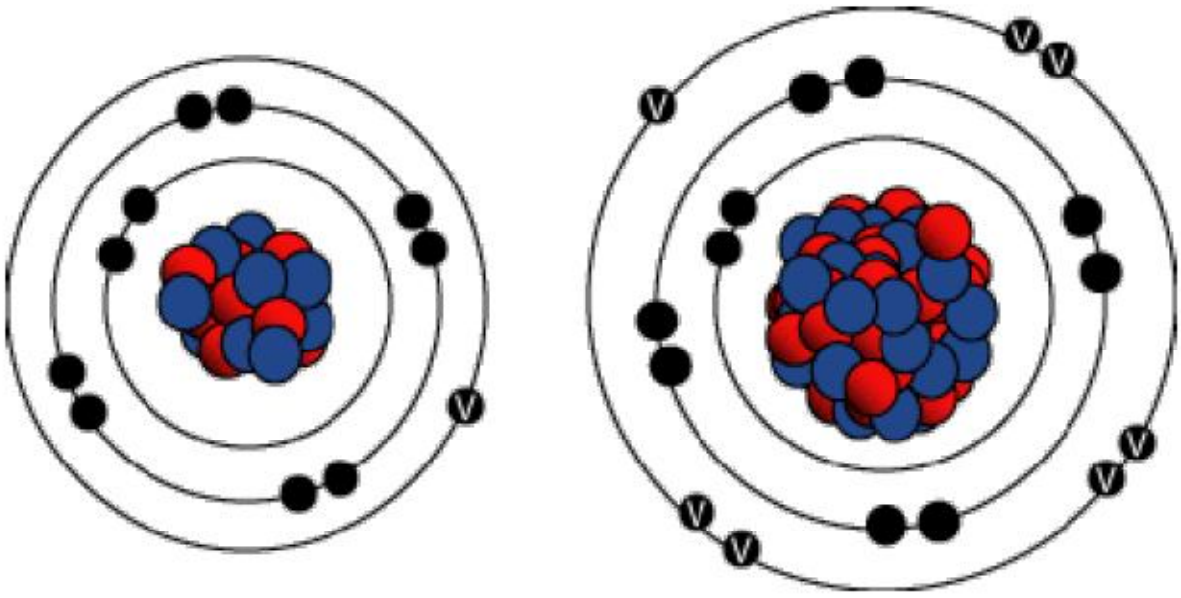
The nucleus is composed of protons and neutrons
Atomic number identifies number of protons in the nucleus
Atomic mass is the sum of masses of protons and neutrons
Electrons orbit the nucleus
Protons and electrons have equal and opposite electrical charge

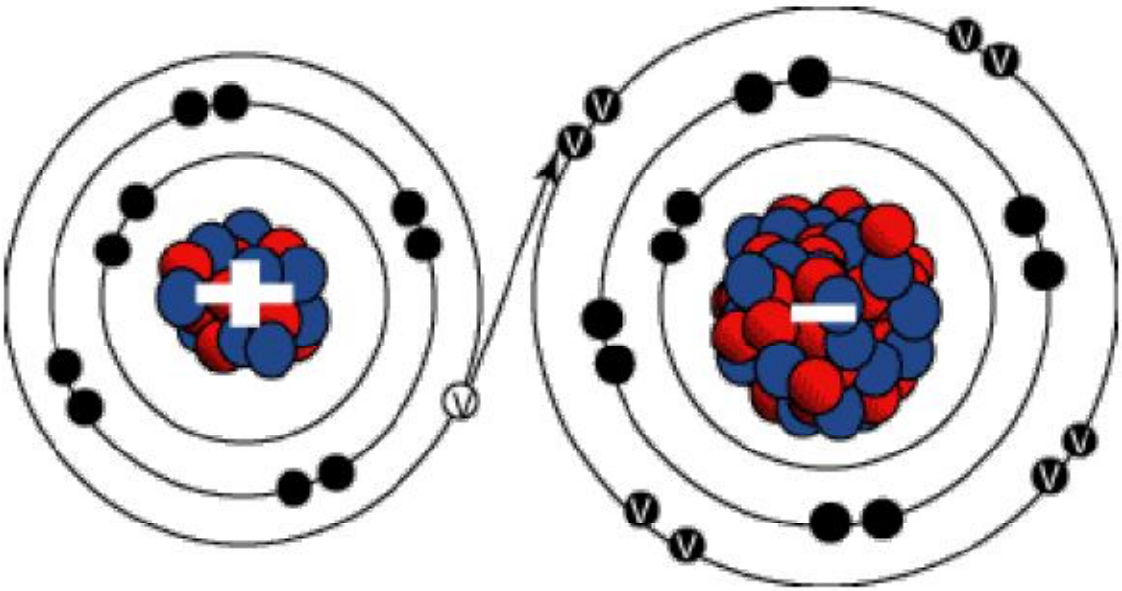
Ionic Bonds

Ionic bonding occurs between charged particles. These may be atoms or groups of atoms, but this discuss will be conducted in terms of single atoms. Ionic bonding occurs between metal atoms and nonmetal atoms. Metals usually have 1, 2, or 3 electrons in their outermost shell. Nonmetals have 5, 6, or 7 electrons in their outer

shell. Atoms with outer shells that are only partially filled are unstable. To become stable, the metal atom wants to get rid of one or more electrons in its outer shell. Losing electrons will either result in an empty outer shell or get it closer to having an empty outer shell. It would like to have an empty outer shell because the next lower energy shell is a stable shell with eight electrons.

Since electrons have a negative charge, the atom that gains electrons becomes a negatively charged ions (aka anion) because it now has more electrons than protons. Alternately, an atom that loses electrons becomes a positively charged ion (aka cations). The particles in an ionic compound are held together because there are oppositely charged particles that are attracted to one another.





The images above schematically show the process that takes place during the formation of an ionic bond between sodium and chlorine atoms. Note that sodium has one valence electron that it would like to give up so that it would become stable with a full outer shell of eight. Also note that chlorine has seven valence electrons and it would like to gain an electron in order to have a full shell of eight. The transfer of the electron causes the previously neutral sodium atom to become a positively charged ion (cation), and the previously neutral chlorine atom to become a negatively charged ion (anion). The attraction for the cation and the anion is called the ionic bond.

Generally, *solid materials* with ionic bonds:

- ✓ are hard because particles cannot easily slide past one another.
- ✓ are good insulators because there are no free electrons or ions (unless dissolved or melted).
- ✓ are transparent because their electrons are not moving from atom to atom and less likely to interact with light photons.
- ✓ are brittle and tend to cleave rather than deform because bonds are strong.
- ✓ have high melting point because ionic bonds are relatively strong.

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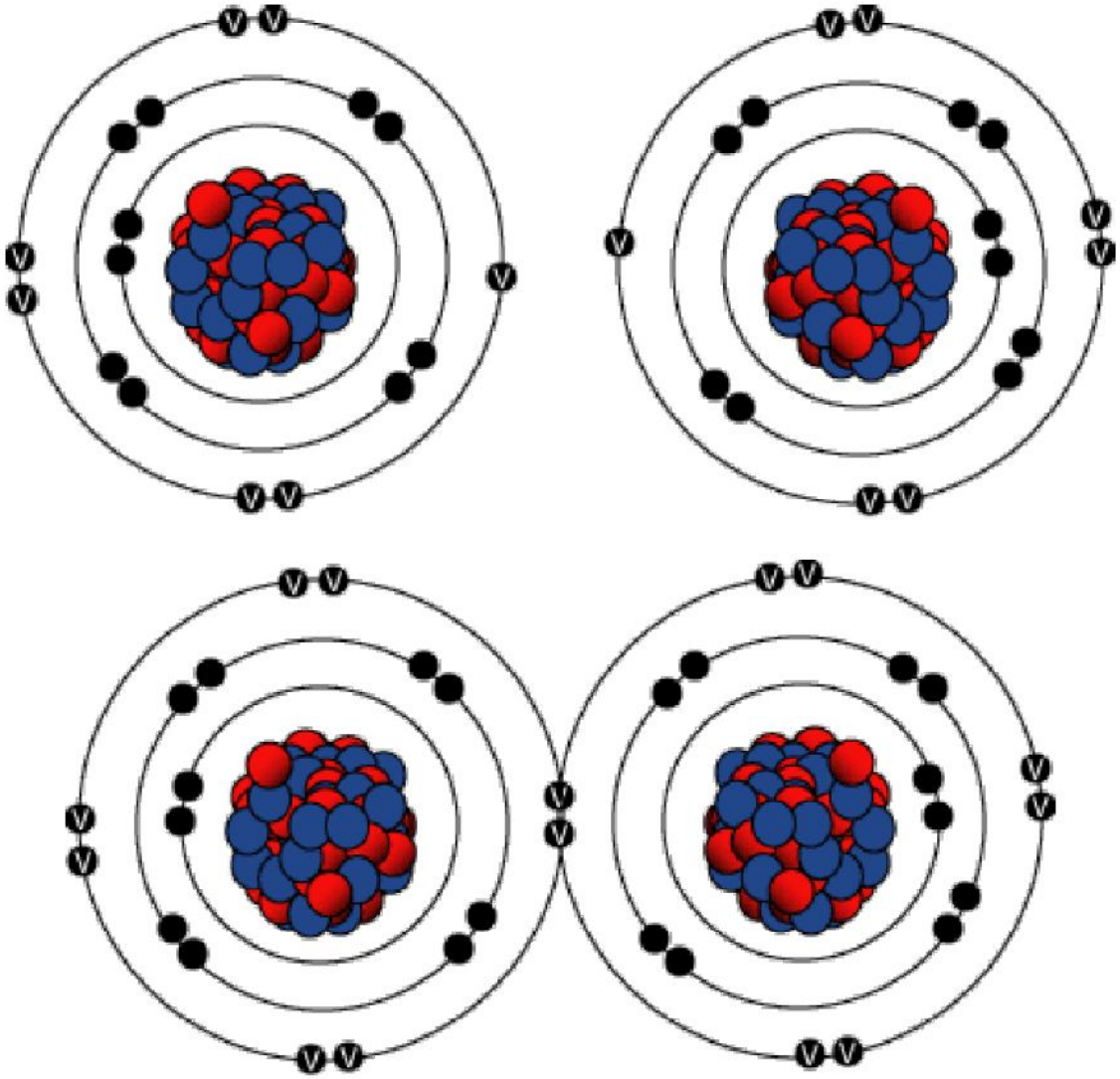
Covalent Bonding

Where a compound only contains nonmetal atoms, a covalent bond is formed by atoms sharing two or more electrons. Nonmetals have 4 or more electrons in their outer shells (except boron). With this many electrons in the outer shell, it would require more energy to remove the electrons than would be gained by making new bonds. Therefore, both the atoms involved share a pair of electrons. Each atom gives one of its outer electrons to the electron pair, which then spends some time with each atom. Consequently, both atoms are held near each other since both atoms have a share in the electrons.

More than one electron pair can be formed with half of the electrons coming from one atom and the rest from the other atom. An important feature of this bond is that the electrons are tightly held and equally shared by the participating atoms. The atoms can be of the same element or different elements. In each molecule, the bonds between the atoms are strong but the bonds between molecules are usually weak. This makes many solid materials with covalent bonds brittle. Many ceramic materials have covalent bonds.

Compounds with covalent bonds may be solid, liquid or gas at room temperature depending on the number of atoms in the compound. The more atoms in each molecule, the higher a compound's melting and boiling temperature will be. Since most covalent compounds contain



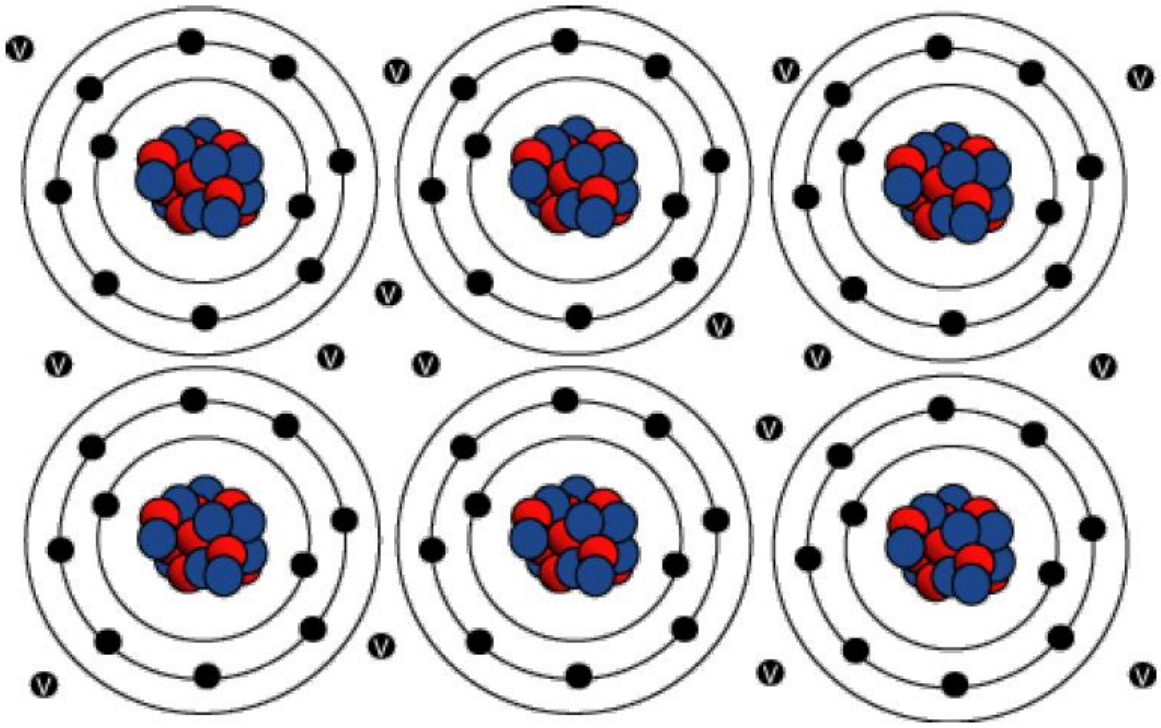
only a few atoms and the forces between molecules are weak, most covalent compounds have low melting and boiling points. However, some, like carbon compounds, can be very large. An example is the diamond in which carbon atoms each share four electrons to form giant lattices.

Some Common Features of Materials with Covalent Bonds:

- ✓ Low enthalpies of fusion and vaporization
- ✓ Good insulators
- ✓ Solids can be soft or brittle
- ✓ If brittle often transparent and cleave rather than deform.

Metallic Bonding

A common characteristic of metallic elements is they contain only one to three electrons in the outer shell. When an element has only one,two or three valence electrons (i.e. electrons in the outer shell), the bond between these electrons and the nucleus is relatively weak. So, for example, when aluminum atoms are grouped together in a block of metal, the outer electrons leave individual atoms to become part of common “electron cloud.” In this arrangement, the valence electrons have considerable mobility and are able to conduct heat and electricity easily. Also, the delocalized nature of the bonds, make it possible for the atoms to slide past each other when the metal is deformed instead of fracturing like glass or other brittle material.



Since the aluminum atoms lose three electrons, they end up having a positive charge and are designated Al3+ ions (cations). These ions repel each other but are held together in the block because the negative electrons are attracted to the positively charged ions. A result of the sharing of electrons is the cations arrange themselves in a regular pattern. This regular pattern of atoms is the crystalline structure of metals. In the crystal lattice, atoms are packed closely together to

maximize the strength of the bonds. An actual piece of metal consists of many tiny crystals called grains that touch at grain boundaries.

Some Common Features of Materials with Metallic Bonds:

- ✓ Good electrical and thermal conductors due to their free valence electrons
- ✓ Opaque
- ✓ Relatively ductile

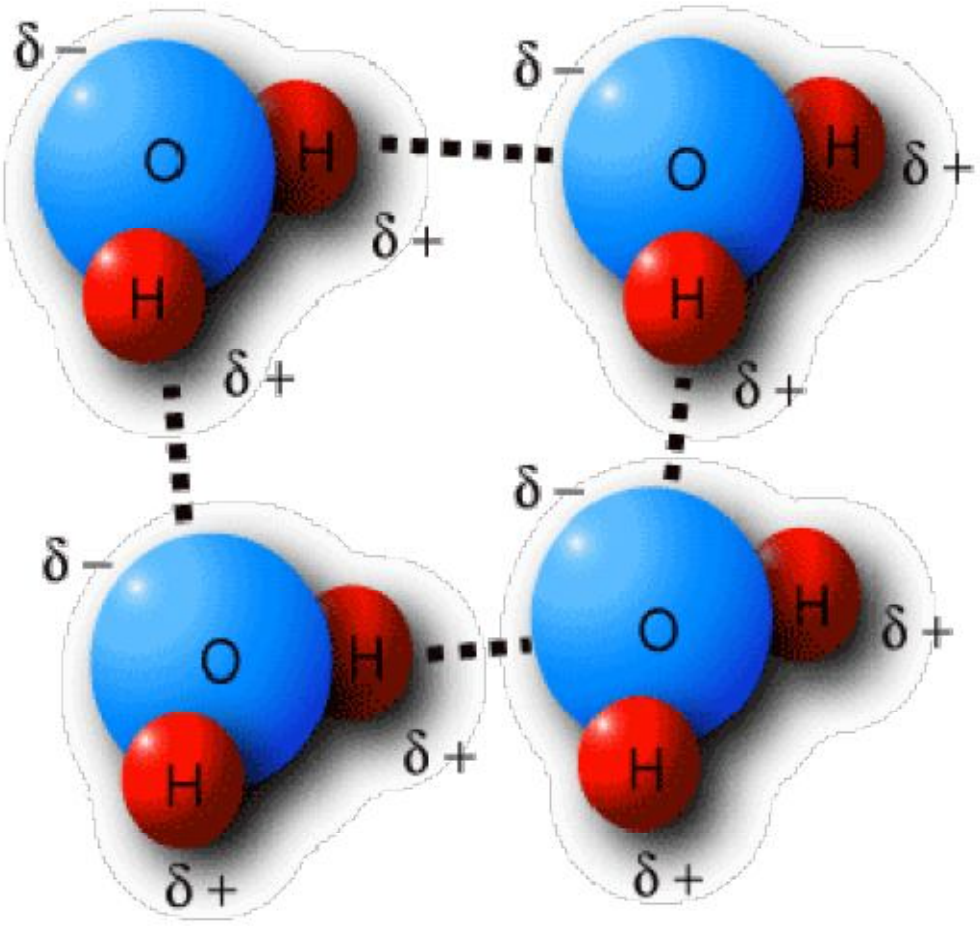
Van der Waals Bond

The van der Waal bonds occur to some extent in all materials but are particularly important in plastics and polymers. These materials are made up of a long string molecules consisting of carbon atoms covalently bonded with other atoms, such as hydrogen, nitrogen, oxygen, fluorine. The covalent bonds within the molecules are very strong and rupture only under extreme conditions. The bonds between the molecules that allow sliding and rupture to occur are called van der Waal forces.

When ionic and covalent bonds are present, there is some imbalance in the electrical charge of the molecule. Take water as an example. Research has determined the hydrogen atoms are bonded to the oxygen atoms at an angle of 104.5°. This angle produces a positive polarity at the hydrogen-rich end of the molecule and a negative polarity at the other end. A result of this charge imbalance is that water molecules are attracted to each other. This is the force that holds the molecules together in a drop of water.

This same concept can be carried on to plastics, except that as molecules become larger, the van der Waal forces between molecules also increases. For example, in polyethylene the molecules are composed of hydrogen and carbon atoms in the same ratio as ethylene gas. But there are more of each type of atom in the polyethylene molecules and as the number of atoms in a molecule increases, the matter passes from a gas to a liquid and finally to a solid.

Polymers are often classified as being either a thermoplastic or a thermosetting material. Thermoplastic materials can be easily remelted for forming or recycling and thermosetting material cannot be easily remelted. In thermoplastic materials consist of long chainlike molecules. Heat can be used to break the van der Waal forces between the molecules and change the form of the material from a solid to a liquid. By contrast, thermosetting materials have a three-dimensional network of covalent bonds. These bonds cannot be easily broken by heating and, therefore, can not be remelted and formed as easily as thermoplastics.

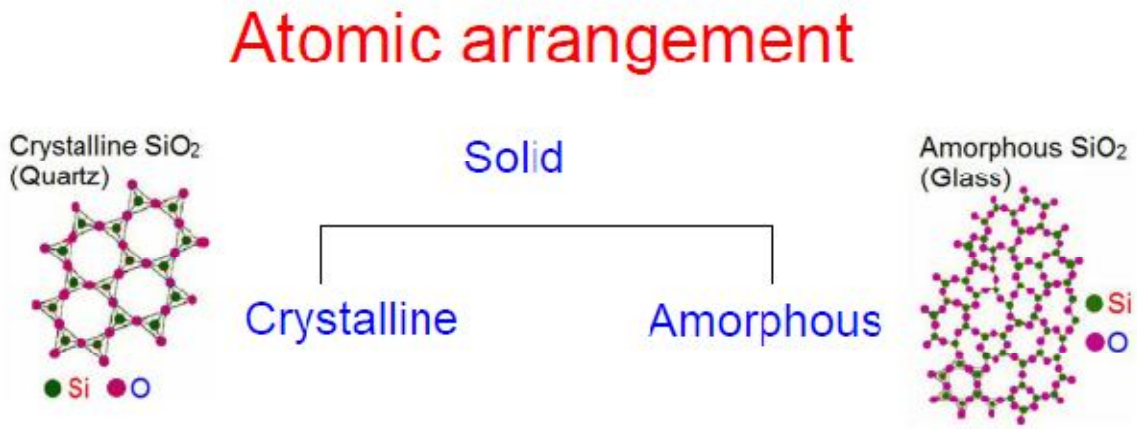


Solid State Structure

In the previous pages, some of the mechanisms that bond together the multitude of individual atoms or molecules of a solid material were discussed. These forces may be primary chemical bonds, as in metals and ionic solids, or they may be secondary van der Waals' forces of solids, such as in ice, paraffin wax and most polymers. In solids, the way the atoms or molecules arrange themselves contributes to the appearance and the properties of the materials.

Atoms can be gathered together as an aggregate through a number of different processes, including condensation, pressurization, chemical reaction, electrodeposition, and melting. The process usually determines, at least initially, whether the collection of atoms will take to form of a gas, liquid or solid. The state usually changes as its temperature or pressure is changed. Melting is the process most often used to form an aggregate of atoms. When the temperature of a melt is

lowered to a certain point, the liquid will form either a crystalline solid or and amorphous solid.



Crystal Structure

Crystal structures may be conveniently specified by describing the arrangement within the solid of a small representative group of atoms or molecules, called the 'unit cell.' By multiplying identical unit cells in three directions, the location of all the particles in the crystal is determined. In nature, 14 different types of crystal structures or lattices are found. The simplest crystalline unit cell to picture is the cubic, where the atoms are lined up in a square, 3D grid. The unit cell is simply a box with an atom at each corner. Simple cubic crystals are relatively rare, mostly because they tend to easily distort. However, many crystals form body-centered-cubic (bcc) or face-centered-cubic (fcc) structures, which are cubic with either an extra atom centered in the cube or centered in each face of the cube. Most metals form bcc, fcc or Hexagonal Close Packed (hpc) structures; however, the structure can change depending on temperature. These three structures will be discussed in more detail on the following page.

Crystalline structure is important because it contributes to the properties of a material. For example, it is easier for planes of atoms to slide by each other if those planes are closely packed. Therefore, lattice structures with closely packed planes allow more plastic deformation than those that are not closely packed. Additionally, cubic lattice structures allow slippage to occur more easily than non-cubic lattices. This is because their symmetry provides closely packed planes in several directions. A face-centered cubic crystal structure will exhibit more ductility (deform more readily under load before breaking) than a body-centered cubicstructure. The bcc lattice, although cubic, is not closely packed and forms

strong metals. Alphairon and tungsten have the bcc form. The fcc lattice is both cubic and closely packed and forms more ductile materials. Gamma-iron, silver, gold, and lead have fcc structures. Finally, HCP lattices are closely packed, but not cubic. HCP metals like cobalt and zinc are not as ductile as the fcc metals.

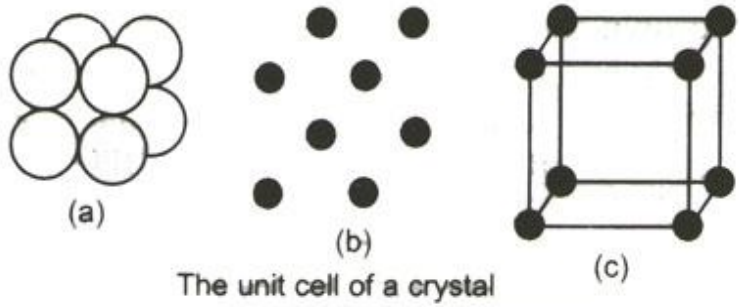
Crystal Lattice is used to represent a three-dimensional periodic array of points coinciding with atom positions.

Unit cell is smallest repeatable entity that can be used to completely represent a crystal structure. It is the building block of crystal structure.

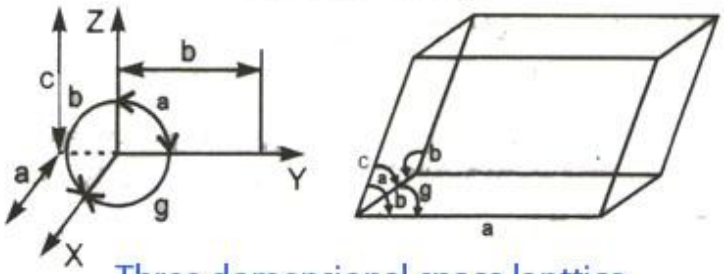
Space Lattice

"A space lattice is an array of points showing how particles (atoms, ions or molecules) are arranged at different sites in three dimensional spaces."

A crystal is a three dimensional design in which identical points form a 3-dimensional network of cells each representing the unit and through which whole crystal can be built up. The lattice points can be connected by a regular network of lines in various ways. Thus the lattice is broken up into a number of unit cells. This is done by connecting the points by a regular network of lines The unit cell may be defined as, *"the smallest repeating unit in space lattice which, when repeated over again, results in a crystal of the given substance".*



The unit cell of a crystal



Three domensional space lanttice

Therefore space lattice of a crystal has been likened to a wall-paper on which a single pattern is continuously repeated. Each unit cell requires two vectors a and b

for its description. A three dimensional space lattice can be similarly divided into unit cells described by three vectors. The exact location of particles in a unit cell can be obtained by X-ray diffraction. It should be understood that the choice of unit cell is by no means unique. There are various ways in which a cell can be drawn in a unique space lattice. However, it is usually convenient to choose a parallelopipe whose edges are parallel with the crystallographic axes (a, b and c) and with the

Bravais lattices

When the crystal systems are combined with the various possible lattice centerings, we arrive at the Bravais lattices. They describe the geometric arrangement of the lattice points, and thereby the translational symmetry of the crystal. In three dimensions, there are 14 unique Bravais lattices that are distinct from one another in the translational symmetry they contain. All crystalline materials recognized until now (not including quasicrystals) fit in one of these arrangements. The fourteen three-dimensional lattices, classified by crystal system, are shown above. The Bravais lattices are sometimes referred to as space lattices.

The crystal structure consists of the same group of atoms, the basis, positioned around each and every lattice point. This group of atoms therefore repeats indefinitely in three dimensions according to the arrangement of one of the 14 Bravais lattices. The characteristic rotation and mirror symmetries of the group of atoms, or unit cell, is described by its crystallographic point group.

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 SiO2 (quartz) is still apparent in amorphous SiO2 (silica glass.)

Crystalline Solids

More than 90% of naturally occurring and artificially prepared solids are crystalline. Minerals, sand, clay, limestone, metals, carbon (diamond and graphite), salts (NaCl, KCl etc.), all have crystalline structures. A crystal is a regular, repeating arrangement of atoms or molecules. The majority of solids, including all metals, adopt a crystalline arrangement because the amount of stabilization achieved by anchoring interactions between neighboring particles is at its greatest when the particles adopt regular (rather than random) arrangements. In the crystalline arrangement, the particles pack efficiently together to minimize the total intermolecular energy. The regular repeating pattern that the atoms arrange in is called the crystalline lattice. The scanning tunneling microscope (STM) makes it possible to image the electron cloud associated individual atoms at the surface of a material. Below is an STM image of a platinum surface showing the regular alignment of atoms.

Amorphous Solids

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 supercooled liquids because their molecules are arranged in a random manner some what as in the liquid state. For example, glass is commonly made from silicon dioxide or quartz sand, which has a crystalline structure. When the sand is melted and the liquid is cooled rapidly enough to avoid crystallization, an amorphous solid called a glass is formed. Amorphous solids do not show a sharp phase change from solid to liquid at a definite melting point, but rather soften gradually when they are heated. The physical properties of amorphous solids are identical in all directions along any axis so they are said to have isotropic properties, which will be discussed in more detail later

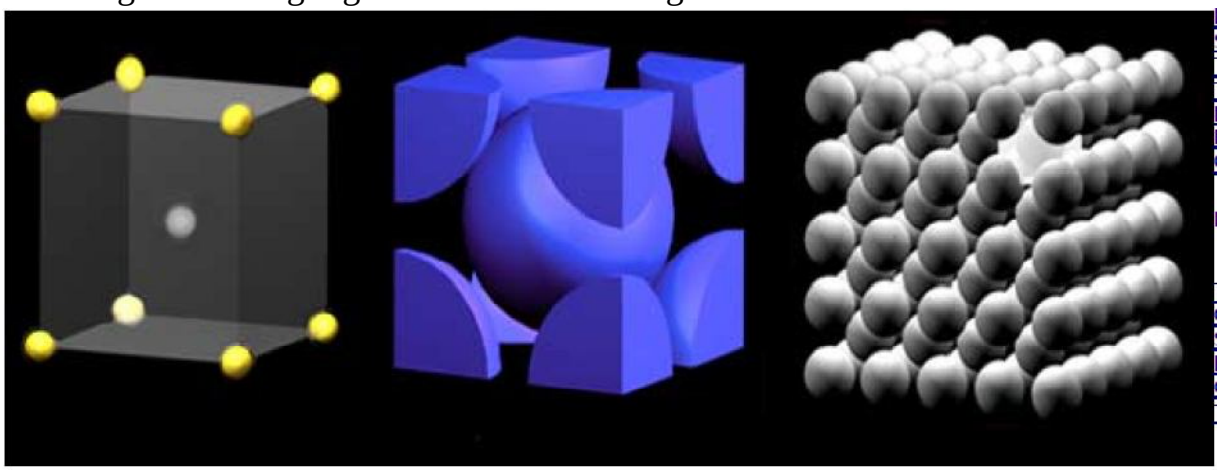
Primary Metallic Crystalline Structures

As pointed out on the previous page, there are 14 different types of crystal unit cell structures or lattices are found in nature. However most metals and many other solids have unit cell structures described as body center cubic (bcc), face centered cubic (fcc) or Hexagonal Close Packed (hcp). Since these structures are most common, they will be discussed in more detail.

Body-Centered Cubic (BCC) Structure

The body-centered cubic unit cell has atoms at each of the eight corners of a cube (like the cubic unit cell) plus one atom in the center of the cube (left image below). Each of the corner atoms is the corner of another cube so the corner atoms are

shared among eight unit cells. It is said to have a coordination number of 8. The bcc unit cell consists of a net total of two atoms; one in the center and eight eighths from corners atoms as shown in the middle image below (middle image below).
The image below highlights a unit cell in a larger section of the lattice.

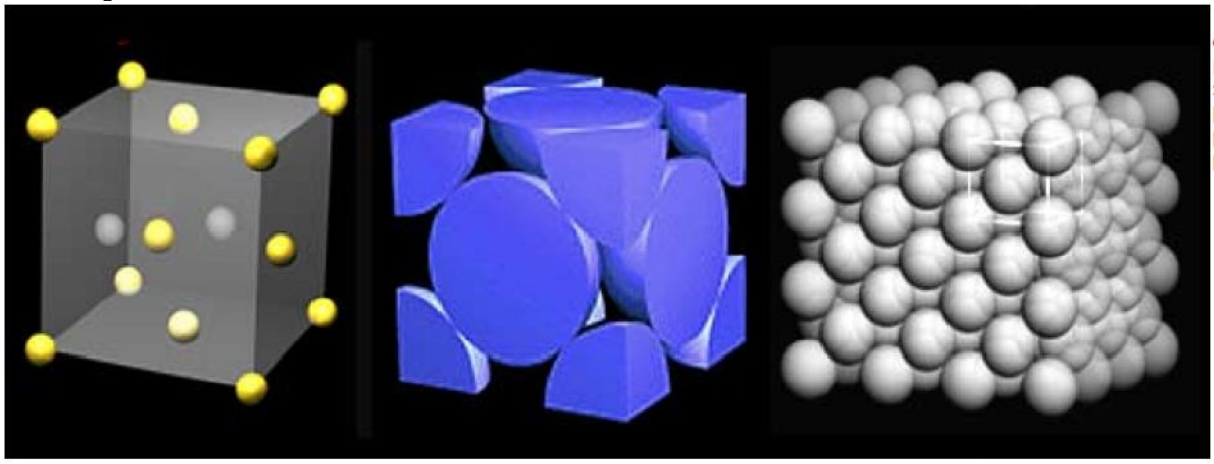


The bcc arrangement does not allow the atoms to pack together as closely as the fcc or hcp arrangements. The bcc structure is often the high temperature form of metals that are close-packed at lower temperatures. The volume of atoms in a cell per the total volume of a cell is called the packing factor. The bcc unit cell has a packing factor of 0.68.
Some of the materials that have a bcc structure include lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten. Metals which have a bcc structure are usually harder and less malleable than close-packed metals such as gold. When the metal is deformed, the planes of atoms must slip over each other, and this is more difficult in the bcc structure. It should be noted that there are other important mechanisms for hardening materials, such as introducing impurities or defects which make slipping more difficult. These hardening mechanisms will be discussed latter.

Face Centered Cubic FCC Structure

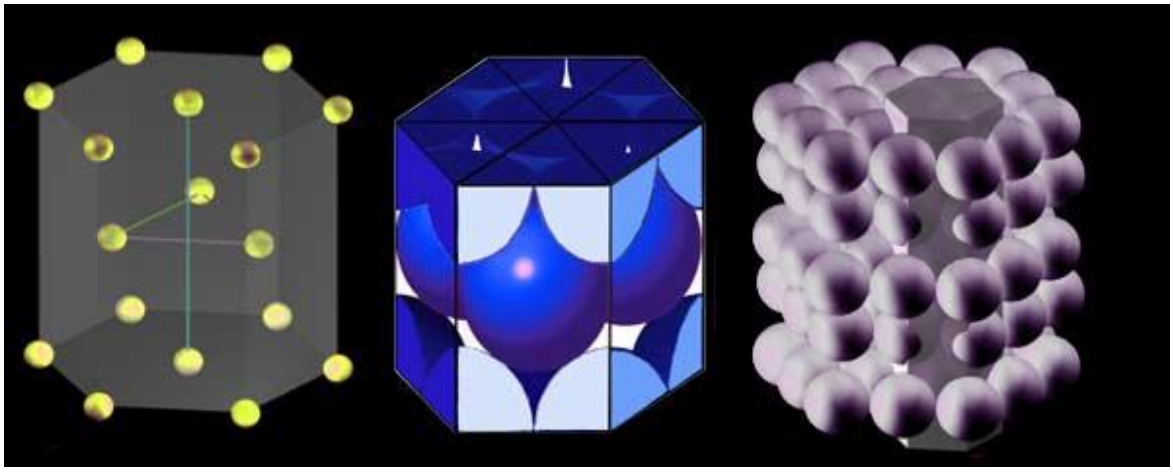
The face centered cubic structure has atoms located at each of the corners and the centers of all the cubic faces (left image below). Each of the corner atoms is the corner of another cube so the corner atoms are shared among eight unit cells. Additionally, each of its six face centered atoms is shared with an adjacent atom. Since 12 of its atoms are shared, it is said to have a coordination number of 12. The fcc unit cell consists of a net total of four atoms; eight eighths from corners atoms and six halves of the face atoms as shown in the middle image above. The image below highlights a unit cell in a larger section of the lattice.

In the fcc structure (and the hcp structure) the atoms can pack closer together than they can in the bcc structure. The atoms from one layer nest themselves in the empty space between the atoms of the adjacent layer. To picture packing arrangement, imagine a box filled with a layer of balls that are aligned in columns and rows. When a few additional balls are tossed in the box, they will not balance directly on top of the balls in the first layer but instead will come to rest in the pocket created between four balls of the bottom layer. As more balls are added they will pack together to fill up all the pockets. The packing factor (the volume of atoms in a cell per the total volume of a cell) is 0.74 for fcc crystals. Some of the metals that have the fcc structure include aluminum, copper, gold, iridium, lead, nickel, platinum and silver.



Hexagonal Close Packed (HCP) Structure

Another common close packed structure is the hexagonal close pack. The hexagonal structure of alternating layers is shifted so its atoms are aligned to the gaps of the preceding layer. The atoms from one layer nest themselves in the empty space between the atoms of the adjacent layer just like in the fcc structure. However, instead of being a cubic structure, the pattern is hexagonal. (See image below.) The difference between the HCP and FCC structure is discussed later in this section.



The hcp structure has three layers of atoms. In each the top and bottom layer, there are six atoms that arrange themselves in the shape of a hexagon and a seventh atom that sits in the middle of the hexagon. The middle layer has three atoms nestle in the triangular "grooves" of the top and bottom plane. Note that there are six of these "grooves" surrounding each atom in the hexagonal plane, but only three of them can be filled by atoms.

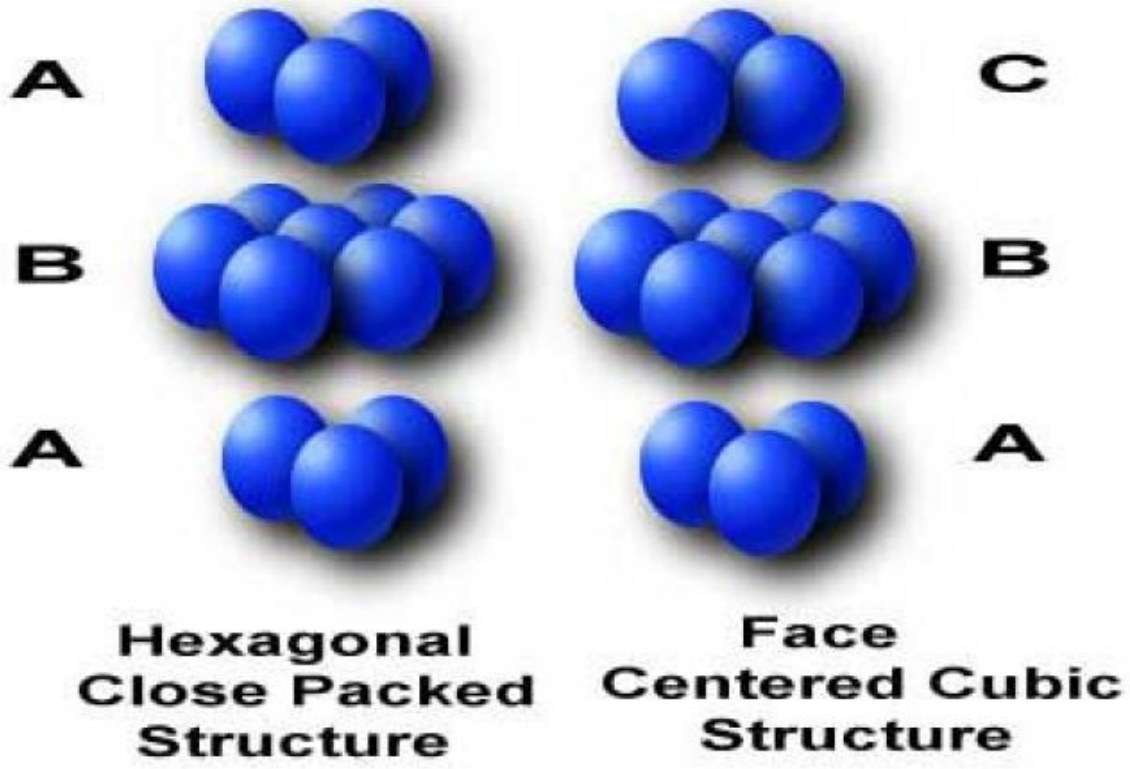
As shown in the middle image above, there are six atoms in the hcp unit cell. Each of the 12 atoms in the corners of the top and bottom layers contribute 1/6 atom to the unit cell, the two atoms in the center of the hexagon of both the top and bottom layers each contribute atom and each of the three atom in the middle layer contribute 1 atom. The image on the right above attempts to show several hcp unit cells in a larger lattice.

The coordination number of the atoms in this structure is 12. There are six nearest neighbors in the same close packed layer, three in the layer above and three in the layer below. The packing factor is 0.74, which is the same as the fcc unit cell. The hcp structure is very common for elemental metals and some examples include beryllium, cadmium, magnesium, titanium, zinc and zirconium.

Similarities and Difference Between the FCC and HCP Structure

The face centered cubic and hexagonal close packed structures both have a packing factor of 0.74, consist of closely packed planes of atoms, and have a coordination number of 12. The difference between the fcc and hcp is the stacking sequence. The hcp layers cycle among the two equivalent shifted positions whereas the fcc layers cycle between three positions. As can be seen in the image, the hcp structure contains only two types of planes with an alternating ABAB arrangement. Notice how the atoms of the third plane are in exactly the same position as the atoms in the first plane. However, the fcc structure contains three types of planes with a ABCABC arrangement. Notice how the atoms in rows A and C are no longer

aligned. Remember that cubic lattice structures allow slippage to occur more easily than non-cubic lattices, so hcp metals are not as ductile as the fcc metals.



The table below shows the stable room temperature crystal structures for several elemental metals.

Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431
Cadmium	HCP	0.1490
Chromium	BCC	0.1249
Cobalt	HCP	0.1253
Copper	FCC	0.1278
Gold	FCC	0.1442
Iron (Alpha)	BCC	0.1241
Lead	FCC	0.1750
Magnesium	HCP	0.1599
Molybdenum	BCC	0.1363
Nickel	FCC	0.1246
Platinum	FCC	0.1387
Silver	FCC	0.1445
Tantalum	BCC	0.1430
Titanium (Alpha)	HCP	0.1445

Tungsten	BCC	0.1371
Zinc	HCP	0.1332

A nanometer (nm) equals 10^{-9} meter or 10 Angstrom units.

Miller Indices: A system of notation is required to identify particular direction(s) or plane(s) to characterize the arrangement of atoms in a unit cell

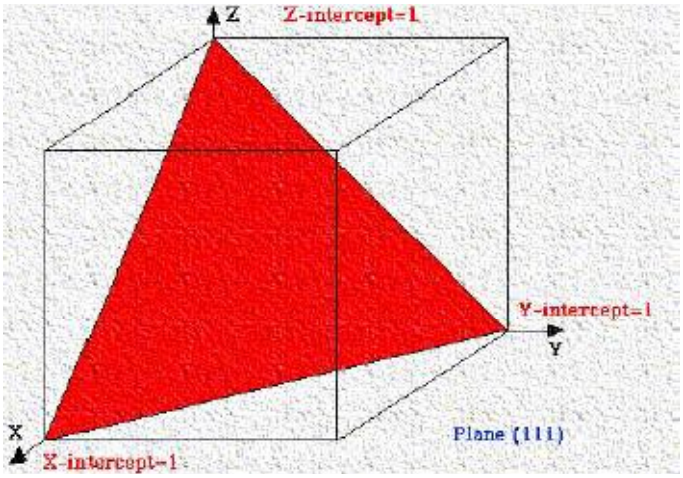
Rules for Miller Indices (Planes)

- ✓ Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
- ✓ Take the reciprocals
- ✓ Clear fractions
- ✓ Reduce to lowest terms
- ✓ For example, if the x-, y-, and z- intercepts 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**)**

Thus, the Miller indices are 3,6,2. If a plane is parallel to an axis, its intercept is at infinity and its Miller index is zero. A generic Miller index is denoted by *(hkl)*. A family of planes is represented by {hkl} 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!

Miller Indices - Direction

- ➢ 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 terms of 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>



Some General Principles

- If a Miller index is zero, the plane is parallel to that axis.
- The smaller a Miller index, the more nearly parallel the plane is to the axis.
- The larger a Miller index, the more nearly perpendicular a plane is to that axis.
- Multiplying or dividing a Miller index by a constant has no effect on the orientation of the plane
- Miller indices are almost always small.

Why Miller Indices?

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 face with a similar stacking pattern, regardless of the crystal class of the crystal. Face 111 always steps the same way regardless of crystal system.

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Crystal Defects

A perfect crystal, with every atom of the same type in the correct position, does not exist. All crystals have some defects. Defects contribute to the mechanical properties of metals. In fact, using the term “defect” is sort of a misnomer since these features are commonly intentionally used to manipulate the mechanical properties of a material. Adding alloying elements to a metal is one way of introducing a crystal defect. Nevertheless, the term “defect” will be used, just keep in mind that crystalline defects are not always bad. There are basic classes of crystal defects:

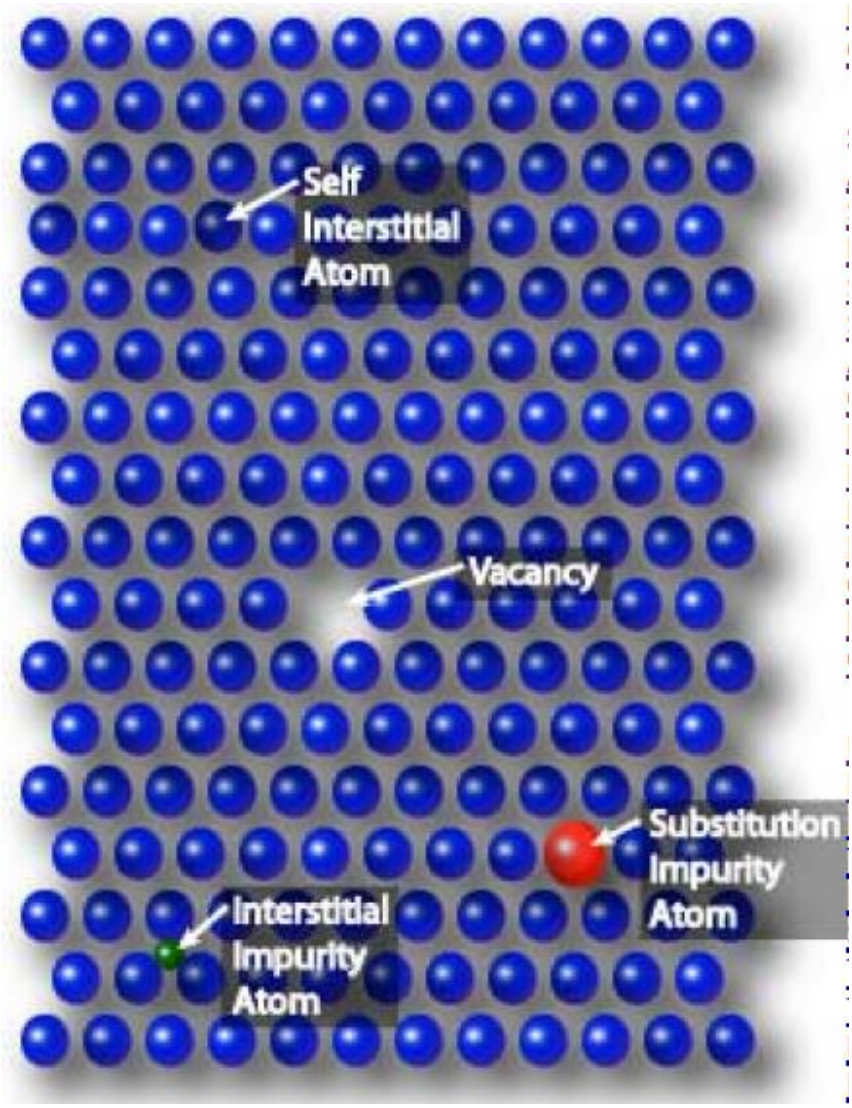
- ✓ **Point defects**, which are places where an atom is missing or irregularly placed in the lattice structure. Point defects include lattice vacancies, self-interstitial atoms, substitution impurity atoms, and interstitial impurity atoms
- ✓ **Linear defects**, which are groups of atoms in irregular positions. Linear defects are commonly called dislocations.
- ✓ **Planar defects**, which are interfaces between homogeneous regions of the material. Planar defects include grain boundaries, stacking faults and external surfaces.

It is important to note at this point that plastic deformation in a material occurs due to the movement of dislocations (linear defects). Millions of dislocations result for plastic forming operations such as rolling and extruding. It is also important to note that any defect in the regular lattice structure disrupts the motion of dislocation, which makes slip or plastic deformation more difficult. These defects not only include the point and planer defects mentioned above, and also other dislocations. Dislocation movement produces additional dislocations, and when dislocations run into each other it often impedes movement of the dislocations. This drives up the force needed to move the dislocation or, in other words, strengthens the material. Each of the crystal defects will be discussed in more detail in the following pages.

Point defects

Point defects are where an atom is missing or is in an irregular place in the lattice structure. Point defects include self interstitial atoms, interstitial impurity atoms, substitutional atoms and vacancies. A ***self interstitial atom*** is an extra atom that has crowded its way into an interstitial void in the crystal structure. Self interstitial

atoms occur only in low concentrations in metals because they distort and highly stress the tightly packed lattice structure.



A ***substitutional impurity*** atom is an atom of a different type than the bulk atoms, which has replaced one of the bulk atoms in the lattice. Substitutional impurity atoms are usually close in size (within approximately 15%) to the bulk atom. An example of substitutional impurity atoms is the zinc atoms in brass. In brass, zinc atoms with a radius of 0.133 nm have replaced some of the copper atoms, which have a radius of 0.128 nm.

Interstitial impurity atoms are much smaller than the atoms in the bulk matrix. Interstitial impurity atoms fit into the open space between the bulk atoms of the lattice structure. An example of interstitial impurity atoms is the carbon atoms that

are added to iron to make steel. Carbon atoms, with a radius of 0.071 nm, fit nicely in the open spaces between the larger (0.124 nm) iron atoms.

Vacancies are empty spaces where an atom should be, but is missing. They are common, especially at high temperatures when atoms are frequently and randomly change their positions leaving behind empty lattice sites. In most cases diffusion (mass transport by atomic motion) can only occur because of vacancies.

Linear Defects - Dislocations

Dislocations are another type of defect in crystals. Dislocations are areas were the atoms are out of position in the crystal structure. Dislocations are generated and move when a stress is applied. The motion of dislocations allows slip – plastic deformation to occur.

Before the discovery of the dislocation by Taylor, Orowan and Polyani in 1934, no one could figure out how the plastic deformation properties of a metal could be greatly changed by solely by forming (without changing the chemical composition). This became even bigger mystery when in the early 1900's scientists estimated that metals undergo plastic deformation at forces much smaller than the theoretical strength of the forces that are holding the metal atoms together. Many metallurgists remained skeptical of the dislocation theory until the development of the transmission electron microscope in the late 1950's. The TEM allowed experimental evidence to be collected that showed that the strength and ductility of metals are controlled by dislocations.

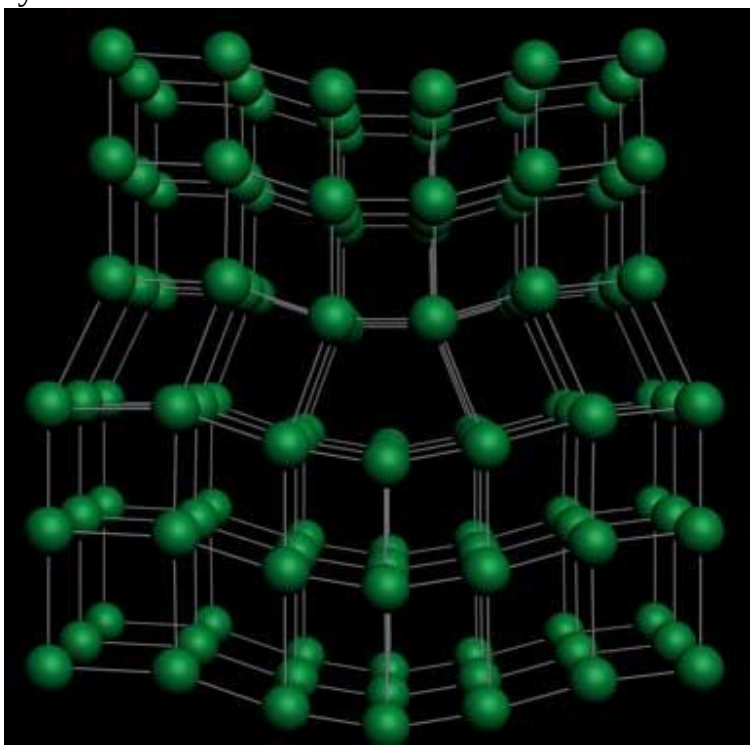
There are two basic types of dislocations, the edge dislocation and the screw dislocation. Actually, edge and screw dislocations are just extreme forms of the possible dislocation structures that can occur. Most dislocations are probably a hybrid of the edge and screw forms but this discussion will be limited to these two types.

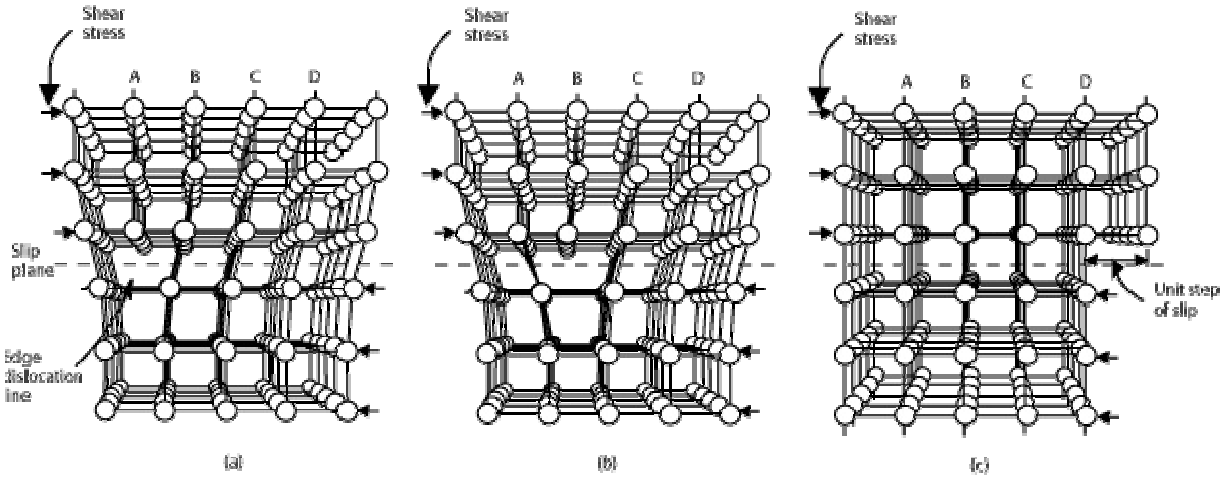
Edge Dislocations

The edge defect can be easily visualized as an extra half-plane of atoms in a lattice. The dislocation is called a line defect because the locus of defective points produced in the lattice by the dislocation lie along a line. This line runs along the top of the extra half-plane. The interatomic bonds are significantly distorted only in the immediate vicinity of the dislocation line.

Understanding the movement of a dislocation is key to understanding why dislocations allow deformation to occur at much lower stress than in a perfect

crystal. Dislocation motion is analogous to movement of a caterpillar. The caterpillar would have to exert a large force to move its entire body at once. Instead it moves the rear portion of its body forward a small amount and creates a hump. The hump then moves forward and eventual moves all of the body forward by a small amount.





As shown in the set of images above, the dislocation moves similarly moves a small amount at a time. The dislocation in the top half of the crystal is slipping one plane at a time as it moves to the right from its position in image (a) to its position in image (b) and finally image (c). In the process of slipping one plane at a time the

dislocation propagates across the crystal. The movement of the dislocation across the plane eventually causes the top half of the crystal to move with respect to the bottom half. However, only a small fraction of the bonds are broken at any given time. Movement in this manner requires a much smaller force than breaking all the bonds across the middle plane simultaneously.

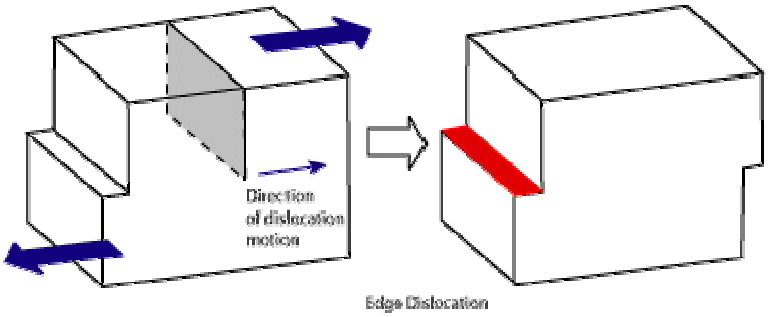
Screw Dislocations

There is a second basic type of dislocation, called screw dislocation. The screw dislocation is slightly more difficult to visualize. The motion of a screw dislocation is also a result of shear stress, but the defect line movement is perpendicular to direction of the stress and the atom displacement, rather than parallel. To visualize a screw dislocation, imagine a block of metal with a shear stress applied across one end so that the metal begins to rip. This is shown in the upper right image. The lower right image shows the plane of atoms just above the rip. The atoms represented by the blue circles have not yet moved from their original position. The atoms represented by the red circles have moved to their new position in the lattice and have reestablished metallic bonds. The atoms represented by the green circles are in the process of moving. It can be seen that only a portion of the bonds are broke at any given time. As was the case with the edge dislocation, movement in this manner requires a much smaller force than breaking all the bonds across the middle plane simultaneously.

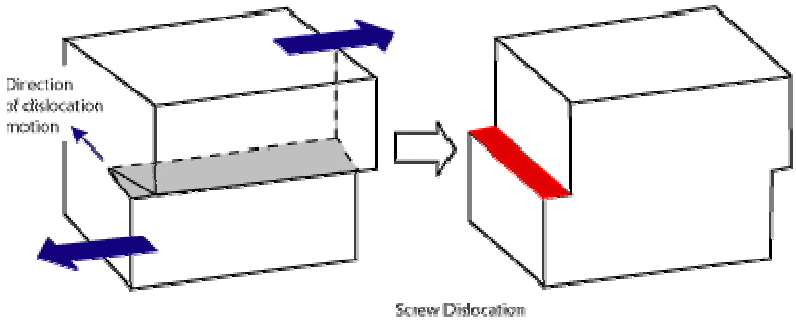
If the shear force is increased, the atoms will continue to slip to the right. A row of the green atoms will find there way back into a proper spot in the lattice (and become red) and a row of the blue atoms will slip out of position (and become green). In this way, the screw dislocation will move upward in the image, which is perpendicular to direction of the stress. Recall that the edge dislocation moves parallel to the direction of stress. As shown in the image below, the net plastic deformation of both edge and screw dislocations is the same, however.

The dislocations move along the densest planes of atoms in a material, because the stress needed to move the dislocation increases with the spacing between the planes. FCC and BCC metals have many dense planes, so dislocations move relatively easy and these materials have high ductility. Metals are strengthened by making it more difficult for dislocations to move. This may involve the introduction of obstacles, such as interstitial atoms or grain boundaries, to “pin” the dislocations. Also, as a material plastically deforms, more dislocations are produced and they will get into each others way and impede movement. This is why strain or work hardening occurs.

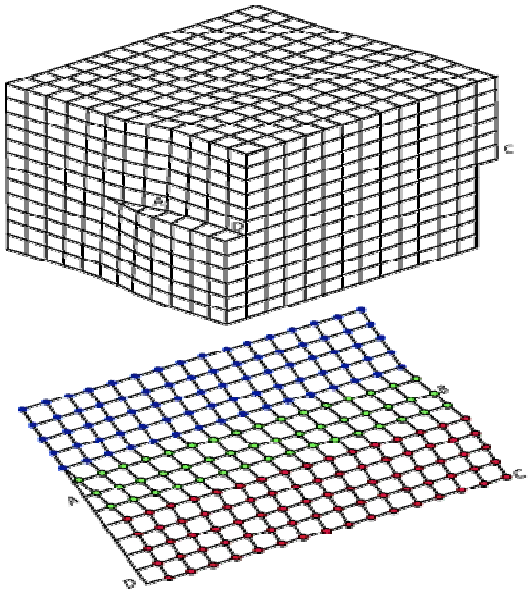
In ionically bonded materials, the ion must move past an area with a repulsive charge in order to get to the next location of the same charge. Therefore, slip is difficult and the materials are brittle. Likewise, the low density packing of covalent materials makes them generally more brittle than metals



Edge Dislocation



Screw Dislocation



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Planar Defects

Stacking Faults and Twin Boundaries

A disruption of the long-range stacking sequence can produce two other common types of crystal defects: 1) a stacking fault and 2) a twin region. A change in the stacking sequence over a few atomic spacings produces a stacking fault whereas a change over many atomic spacings produces a twin region.

A stacking fault is a one or two layer interruption in the stacking sequence of atom planes. Stacking faults occur in a number of crystal structures, but it is easiest to see how they occur in close packed structures. For example, it is know from a previous discussion that face centered cubic (fcc) structures differ from hexagonal close packed (hcp) structures only in their stacking order. For hcp and fcc structures, the first two layers arrange themselves identically, and are said to have an AB arrangement. If the third layer is placed so that its atoms are directly above those of the first (A) layer, the stacking will be ABA. This is the hcp structure, and it continues ABABABAB. However it is possible for the third layer atoms to arrange themselves so that they are in line with the first layer to produce an ABC arrangement which is that of the fcc structure. So, if the hcp structure is going along as ABABAB and suddenly switches to ABABABCABAB, there is a stacking fault present.

Alternately, in the fcc arrangement the pattern is ABCABCABC. A stacking fault in an fcc structure would appear as one of the C planes missing. In other words the pattern would become ABCABCAB_ABCABC.

If a stacking fault does not corrects itself immediately but continues over some number of atomic spacings, it will produce a second stacking fault that is the twin of the first one. For example if the stacking pattern is ABABABAB but switches to ABCABCABC for a period of time before switching back to ABABABAB, a pair of twin stacking faults is produced. The red region in the stacking sequence that goes ABCABCACBACBABCABC is the twin plane and the twin boundaries are the A planes on each end of the highlighted region.

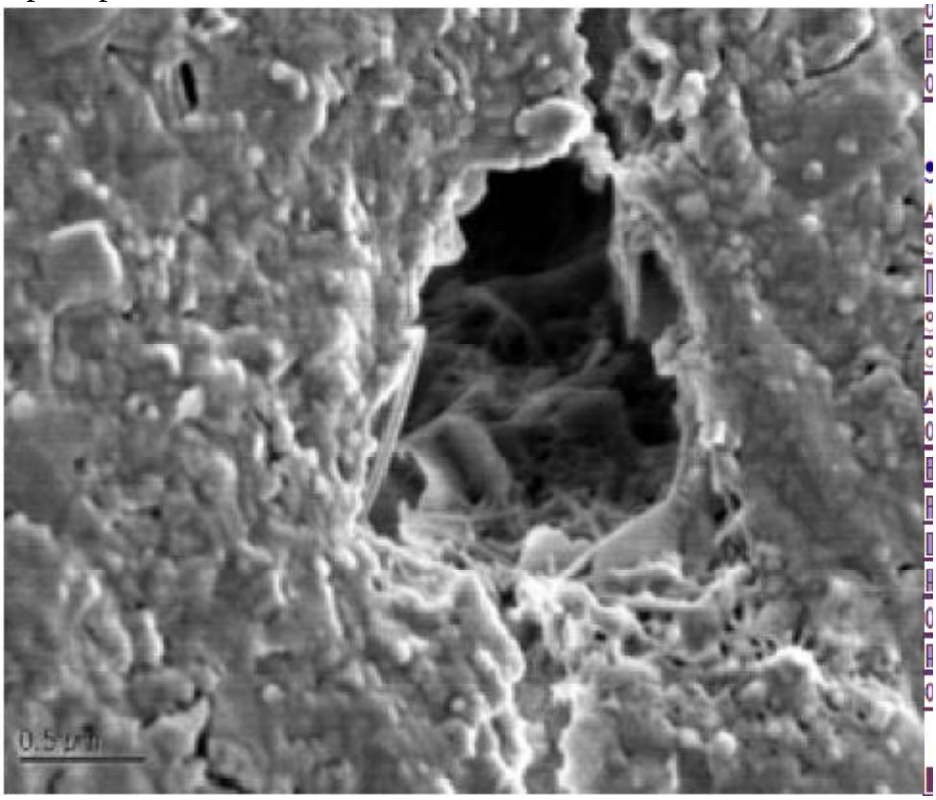
Grain Boundaries in Polycrystals

Another type of planer defect is the grain boundary. Up to this point, the discussion has focused on defects of single crystals. However, solids generally consist of a number of crystallites or grains. Grains can range in size from nanometers to millimeters across and their orientations are usually rotated with respect to neighboring grains. Where one grain stops and another begins is know as a grain boundary. Grain boundaries limit the lengths and motions of dislocations. Therefore, having smaller grains (more grain boundary surface area) strengthens a material. The size of the grains can be controlled by the cooling rate when the

material cast or heat treated. Generally, rapid cooling produces smaller grains whereas slow cooling result in larger grains. For more information, refer to the discussion on solidification.

Bulk Defects

Bulk defects occur on a much bigger scale than the rest of the crystal defects discussed in this section. However, for the sake of completeness and since they do affect the movement of dislocations, a few of the more common bulk defects will be mentioned. Voids are regions where there are a large number of atoms missing from the lattice. The image to the right is a void in a piece of metal.The image was acquired using a Scanning Electron Microscope (SEM). Voids can occur for a number of reasons. When voids occur due to air bubbles becoming trapped when a material solidifies, it is commonly called porosity. When a void occurs due to the shrinkage of a material as it solidifies, it is called cavitation. Another type of bulk defect occurs when impurity atoms cluster together to form small regions of a different phase. The term ‘phase’ refers to that region of space occupied by a physically homogeneous material. These regions are often called precipitates. Phases and precipitates will be discussed in more detail latter.



Atomic packing factor (APF)

Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell

APF = Volume of atom / Volume of unit cell

Planar density

Planar density (PD) refers to density of atomic packing on a particular plane.

Planar density (PD) = Number of atoms on a plane / Area of plane

Linear Density

Linear density (LD) is the number of atoms per unit length along a particular direction

LD = Number of atoms on the direction vector / Length of the direction vector

X-RAY DIFFRACTION: DETERMINATION OF CRYSTAL STRUCTURES

X-ray diffraction (XRD) relies on the dual wave/particle nature of X-rays to obtain information about the structure of crystalline materials. A primary use of the technique is the identification and characterization of compounds based on their diffraction pattern.

The dominant effect that occurs when an incident beam of monochromatic X-rays interacts with a target material is scattering of those X-rays from atoms within the target material. In materials with regular structure (i.e. crystalline), the scattered X-rays undergo constructive and destructive interference. This is the process of diffraction. The diffraction of X-rays by crystals is described by Bragg's Law, $n(\lambda) = 2d \sin(\Theta)$. The directions of possible diffractions depend on the size and shape of the unit cell of the material. The intensities of the diffracted waves depend on the kind and arrangement of atoms in the crystal structure. However, most materials are not single crystals, but are composed of many tiny crystallites in all possible orientations called a polycrystalline aggregate or powder. When a powder with randomly oriented crystallites is placed in an X-ray beam, the beam will see

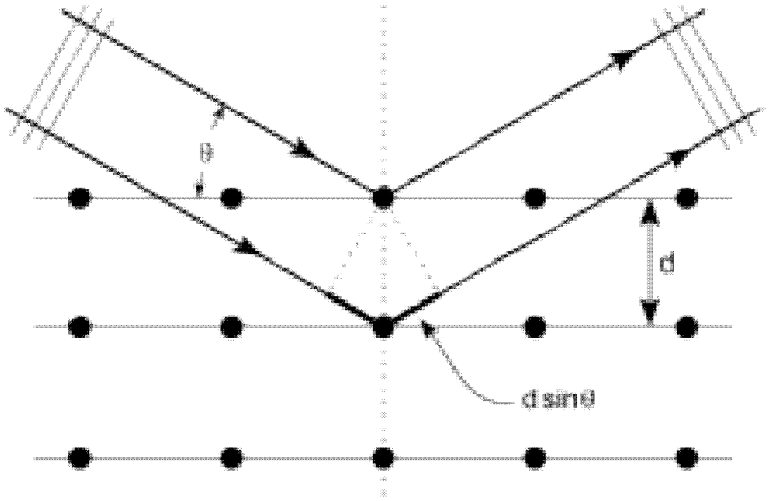
all possible interatomic planes. If the experimental angle is systematically changed, all possible diffraction peaks from the powder will be detected.

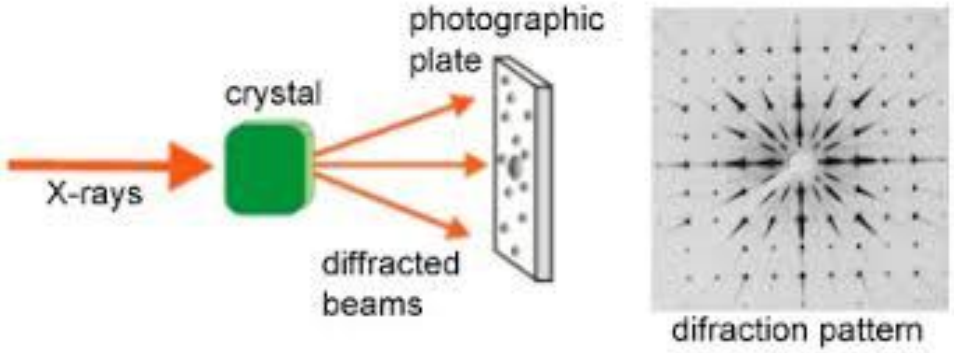
The parafocusing (or Bragg-Brentano) diffractometer is the most common geometry for diffraction instruments.

This geometry offers the advantages of high resolution and high beam intensity analysis at the cost of very precise alignment requirements and carefully prepared samples. Additionally, this geometry requires that the source-to-sample distance be constant and equal to the sample-to-detector distance. Alignment errors often lead to difficulties in phase identification and improper quantification. A mis-positioned sample can lead to unacceptable specimen displacement errors. Sample flatness, roughness, and positioning constraints preclude in-line sample measurement. Additionally, traditional XRD systems are often based on bulky equipment with high power requirements as well as employing high powered X-ray sources to increase X-ray flux on the sample, therefore increasing the detected diffraction signals from the sample. These sources also have large excitation areas, which are often disadvantageous for the diffraction analysis of small samples or small sample features.

Polycapillary X-ray optics can be used to overcome many of these drawbacks and constraints to enhance XRD applications. Polycapillary collimating optics convert a highly divergent beam into a quasi-parallel beam with low divergence. They can be used to form a Parallel Beam XRD instrument geometry which greatly reduces and removes many sources of errors in peak position and intensity inherent to the parafocusing geometry, such as sample position, shape, roughness, flatness, and transparency. Polycapillary focusing optics collect X-rays from a divergent X-ray source and direct them to a small focused beam at the sample surface with diameters as small as tens of micrometers for micro X-ray diffraction applications of small samples or small specimen features. Both types of polycapillary optics direct very high X-ray intensities to the sample surface, such that XRD systems employing optics can use low power X-ray sources, reducing instrument size, cost, and power requirements.

X-ray diffraction using X-ray optics has been applied to many different types of applications including thin film analysis, sample texture evaluation, monitoring of crystalline phase and structure, and investigation of sample stress and strain.





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