

## Chapter 1

# Introductory Remarks

**Crystalline vs. non-crystalline solids:**

**Lattice**

**Unit cell**

**No. of spheres in a unit cell :**

[http://en.wikipedia.org/wiki/Bravais\\_lattice](http://en.wikipedia.org/wiki/Bravais_lattice)

## Bravais lattices

From Wikipedia, the free encyclopedia

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In [geometry](#) and [crystallography](#), a **Bravais lattice**, named after [Auguste Bravais](#), is an infinite set of points generated by a set of discrete [translation](#) operations. A crystal is made up of one or more atoms (the *basis*) which is repeated at each lattice point. The crystal then looks the same when viewed from any of the lattice points. In all, there are 14 possible Bravais lattices that fill three-dimensional space. Related to Bravais lattices are [Crystallographic point groups](#) of which there are 32 and [Space groups](#) of which there are 230. Development of the Bravais lattices

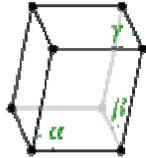
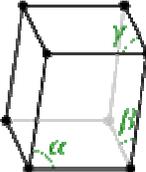
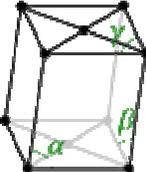
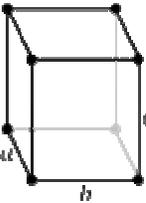
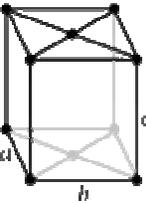
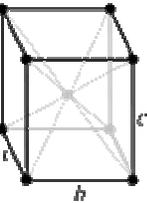
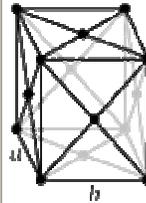
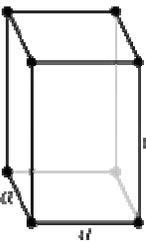
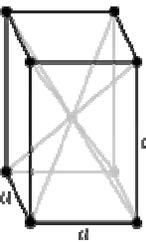
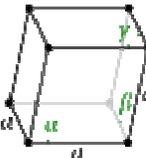
The 14 Bravais lattices are arrived at by combining one of the seven [crystal systems](#) (or axial systems) with one of the lattice centerings.

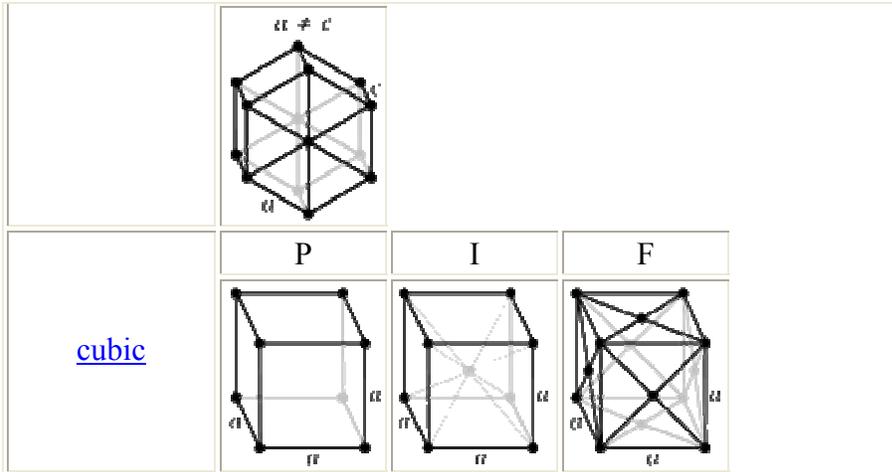
The lattice centerings are:

- Primitive centering (P): lattice points on the cell corners only
- Body centered (I): one additional lattice point at the center of the cell
- Face centered (F): one additional lattice point at center of each of the faces of the cell
- Centered on a single face (A, B or C centering): one additional lattice point at the center of one of the cell faces.

Not all combinations of the crystal systems and lattice centerings are needed to describe the possible lattices. There are in total  $7 \times 6 = 42$  combinations, but it can be shown that several of these are in fact equivalent to each other. For example, the monoclinic I lattice can be described by a monoclinic C lattice by different choice of crystal axes. Similarly,

all A- or B-centered lattices can be described either by a C- or P-centering. This reduces the number of combinations to 14 conventional Bravais lattices, shown in the table below.

Crystal system	Bravais lattices			
<a href="#">triclinic</a>	P $\alpha, \beta, \gamma \neq 90^\circ$ 			
<a href="#">monoclinic</a>	P $\alpha = 90^\circ$ $\beta, \gamma \neq 90^\circ$ 		C $\alpha \neq 90^\circ$ $\beta, \gamma = 90^\circ$ 	
<a href="#">orthorhombic</a>	P $a \neq b \neq c$ 	C $a \neq b \neq c$ 	I $a \neq b \neq c$ 	F $a \neq b \neq c$ 
<a href="#">tetragonal</a>	P $a \neq c$ 	I $a \neq c$ 		
<a href="#">rhombohedral</a> (trigonal)	P $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ 			
<a href="#">hexagonal</a>	P 			



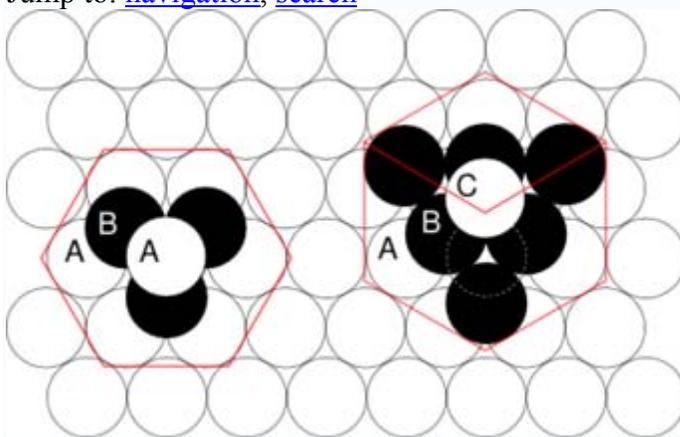
The volume of the unit cell can be calculated by evaluating  $\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}$  where  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  are the lattice vectors. The volumes of the Bravais lattices are given below:

<http://en.wikipedia.org/wiki/Close-packing>

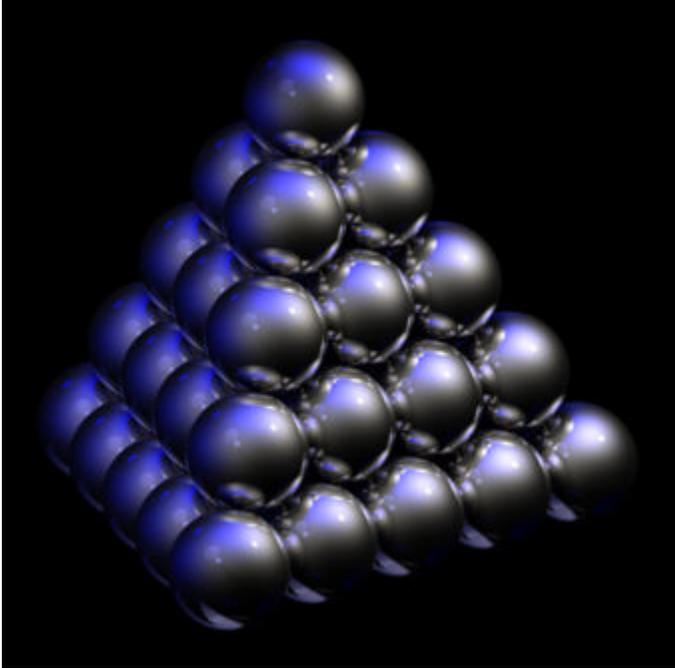
## Close-packing

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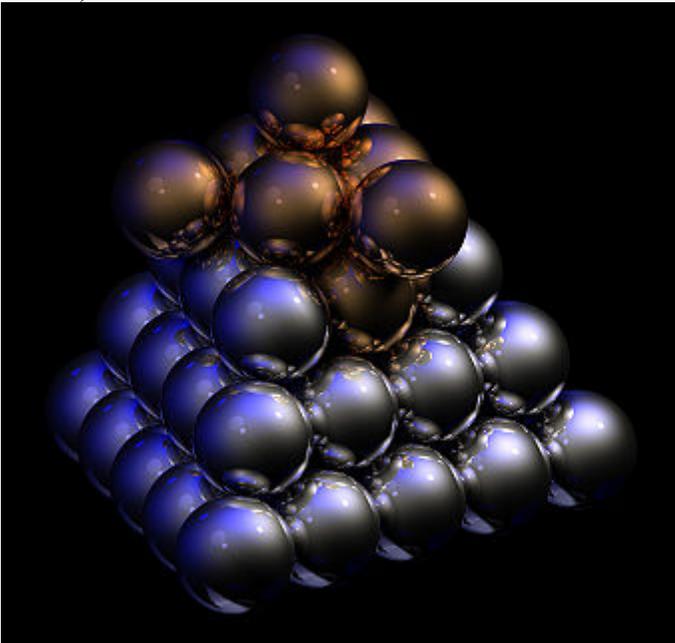
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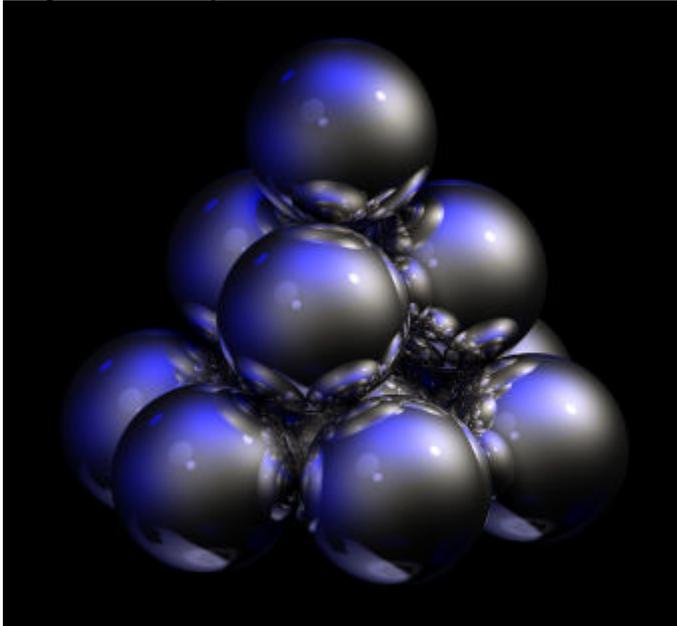
**Fig. 1** Shown above are the HCP lattice (left) and the FCC lattice (right). Note that the two groups shown here are not unit cells that are capable of tessellating in 3D space. These groups do however, readily illustrate the difference between the two lattices.



**Fig. 2** [Thomas Harriot](#) in ca. 1585 first pondered the mathematics of the *cannonball arrangement* or *cannonball stack*, which has an FCC lattice. Note how the two balls facing the viewer in the second tier from the top contact the same ball in the tier below. This does not occur in an HCP lattice (the left organization in *Fig. 1* above, and *Fig. 4* below).



**Fig. 3** Shown here is a modified form of the cannonball stack wherein three extra spheres have been added to show all eight spheres in the top three tiers of the FCC lattice diagrammed in *Fig. 1*.



**Fig. 4** Shown here are all eleven spheres of the HCP lattice illustrated in *Fig. 1*. The difference between this stack and the top three tiers of the cannonball stack all occurs in the bottom tier, which is rotated half the pitch diameter of a sphere ( $60^\circ$ ). Note how the two balls facing the viewer in the second tier from the top do not contact the same ball in the tier below.

**Close-packing** of [spheres](#) is the arranging of an infinite lattice of spheres so that they take up the greatest possible fraction of an infinite 3-dimensional space. [Carl Friedrich Gauss](#) proved that the highest average density that can be achieved by a regular lattice

arrangement is  $\frac{\pi}{3\sqrt{2}} \simeq 0.74048$ . The [Kepler conjecture](#) states that this is the highest density that can be achieved by any arrangement of spheres, either regular or irregular.

There are two regular lattices that achieve this highest average density. They are called face-centered [cubic](#) (FCC) and [hexagonal](#) close-packed (HCP), based on their [symmetry](#). Both are based upon sheets of spheres arranged at the vertices of a triangular tiling; they differ in how the sheets are stacked upon one another. In both arrangements each sphere has twelve neighbors. For every sphere there is one gap surrounded by six spheres (octahedral) and two smaller gaps surrounded by four spheres (tetrahedral).

Relative to a reference layer with positioning A, two more positionings B and C are possible. Every sequence of A, B, and C without immediate repetition of the same one is possible and gives an equally dense packing for spheres of a given radius.

The most regular ones are:

- HCP = ABABABA
- FCC = ABCABCA

Many [crystal](#) structures are based on a close-packing of atoms, or of large ions with smaller ions filling the spaces between them. The cubic and hexagonal arrangements are very close to one another in energy, and it may be difficult to predict which form will be preferred from first principles.

The [coordination number](#) of HCP and FCC is 12 and its [atomic packing factor](#) (APF) is the number mentioned above, 0.74.

### ***Atomic packing factors and examples***

The cubic crystal system is one of the most common crystal systems found in elemental metals, and naturally occurring crystals and minerals. One very useful way to analyse a crystal is to consider the [atomic packing factor](#). In this approach, the amount of space which is filled by the atoms is calculated under the assumption that they are spherical.

**Consider the simple cubic, then:**

$$\text{APF} = 8 \times (1/8) \times (4/3) \times (r^3) \pi / (2r)^3 = 0.52$$

**Examples:**

1) Calculate APF for each of the following unit cells: FCC ,. BCC

2) Which of the following structures is a closest packed arrangement: FCC , BCC , Simple cubic,

### **\*\* *Single-element lattices***

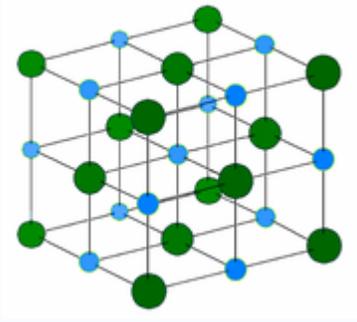
Assuming one atom per lattice point, the atomic packing factor of the **simple cubic system is only 0.524**. Due to its low [density](#), this is a **high energy structure and is rare in nature, but is found in [Polonium](#)** <sup>[1]</sup>.

Similarly, the **body centered structure has APF of 0.680**. The higher density makes this a low energy structure which is fairly common in nature. Examples include [iron](#), [chromium](#), and [tungsten](#).

**Finally, the face centered cubic crystals have a density of 0.741**, a ratio that it shares with several other systems, including [hexagonal close packed](#)

This is the most tightly packed crystal possible with spherical atoms. Due to its low energy, **FCC is extremely common, examples include [lead](#) (for example in [lead\(II\) nitrate](#)), [aluminum](#), [copper](#), and [gold](#)**.

## \*\* Multi-element compounds



The [Sodium Chloride](#) Crystal Structure of type fcc. Each atom has six nearest neighbors, with octahedral geometry. The arrangement of the atoms of each type is known as *cubic close packed* (ccp).

Light blue = Na<sup>+</sup> ([Sodium](#) ion)

Dark green = Cl<sup>-</sup> ([Chloride](#) ion)

When the compound is formed of two elements whose ions are of roughly the same size, they have what is called the **interpenetrating simple cubic** structure, where two atoms of a different type have individual simple cubic crystals. However, the unit cell consists of the atom of one being in the middle of the 8 vertices, structurally resembling body centered cubic. The most common example is [caesium chloride](#) CsCl.

However, if the cation is slightly smaller than the anion (a cation/anion radius ratio of 0.414 to 0.732), the crystal forms a different structure, **interpenetrating FCC**. When drawn separately, both atoms are arranged in an FCC structure. The unit cell for this is shown to the left.

## Tetrahedral and octahedral sites:

Between two layers of ccp structures, there exist Td and Oh sites.

Radius ratio and structure:

Example	$R^+/r^-$ ideal	$R^+/r^-$ actual	C.N	Site	Example
No ccp	0.73	0.93	8		CsCl
CCP	0.41	0.53	6	Oh	NaCl
CCP	0.225	0.402	4	Td	ZnS

Exercise: Use simple geometry to prove the conclusions shown in the above Table.

# Band Theory

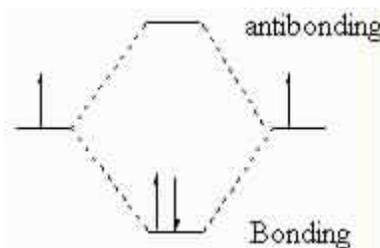
## *Chemist's Point of View*

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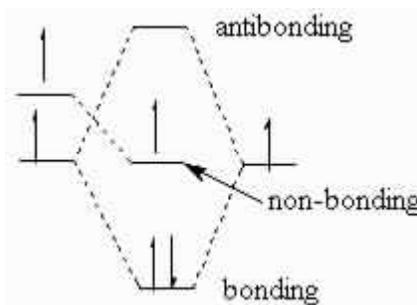
When solids made of an infinite number of atoms are formed, it is a common misconception to consider each atom individually. Rather, we must consider the structure of the solid as a whole. This provides the basis for the description of metals and other types of solids to account for their unique chemical and physical properties.

To fully understand the properties, it is essential to start with molecular orbital theory. In the basic theory, it was assumed that if atoms were brought together, they would form bonding, non-bonding and antibonding orbitals of different energies. These molecular orbitals are described by wave functions. The most important point to come out of the theory is that for  $N$  atomic orbitals in a molecule,  $N$  molecular orbitals must be the outcome.

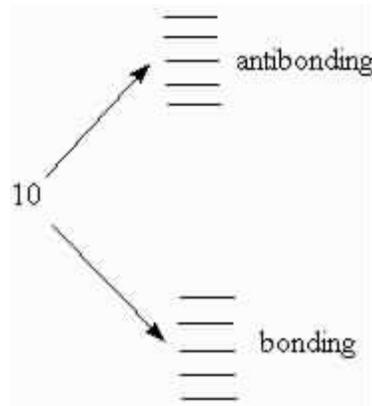
For example, consider a molecule with two atomic orbitals. The result must be that two molecular orbitals will be formed from these atomic orbitals: one bonding and one antibonding, separated by a certain energy.



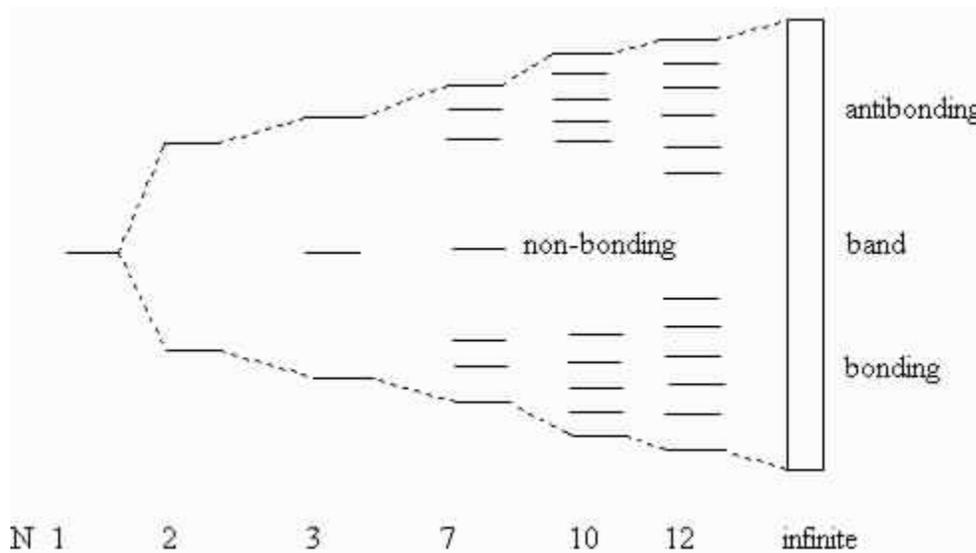
If this is expanded to a molecule with three atoms, assuming 1 atomic orbital for each, then the result must be that 3 molecular orbitals will be formed: one bonding, one non-bonding and one anti-bonding.



Now, let's take it to 10 atoms. This will produce 10 molecular orbitals: 5 bonding and 5 anti-bonding. Now let's take a close look at the separation between each set of orbitals. As the number of molecular orbitals increases, the energy difference between the lowest bonding and the highest antibonding increases, while the space between each individual orbital decreases. As the number of molecular orbitals increases with the number of atoms in a molecule, it will be observed that the spacing between the lowest bonding and highest antibonding orbital will reach a maximum.

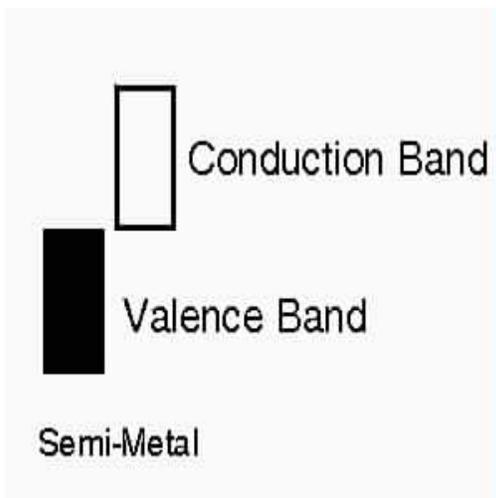
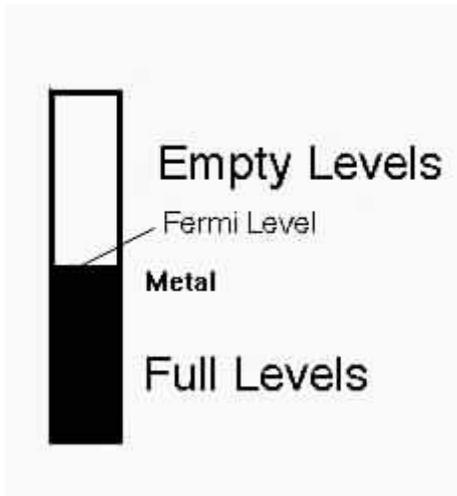


Now consider a metal with an infinite number of atoms. This will form an infinite number of molecular orbitals so close together they blur into one another forming a band. This whole process is shown below.

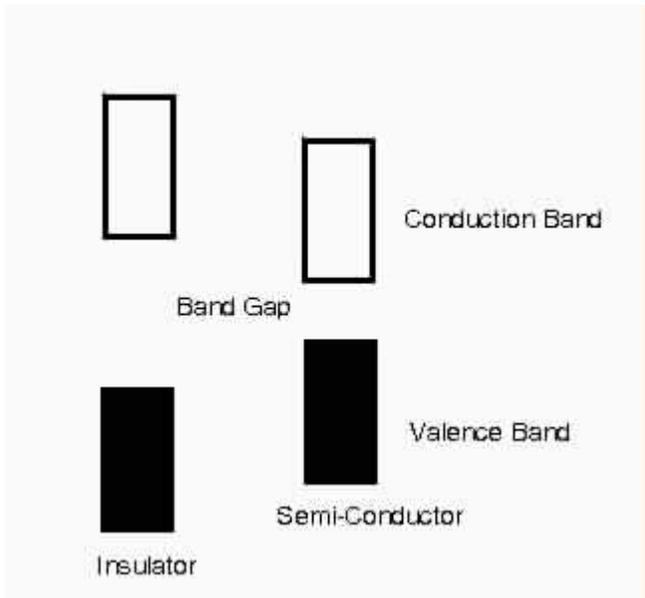
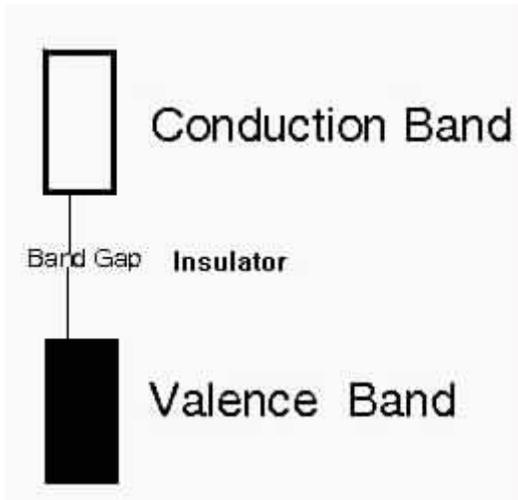


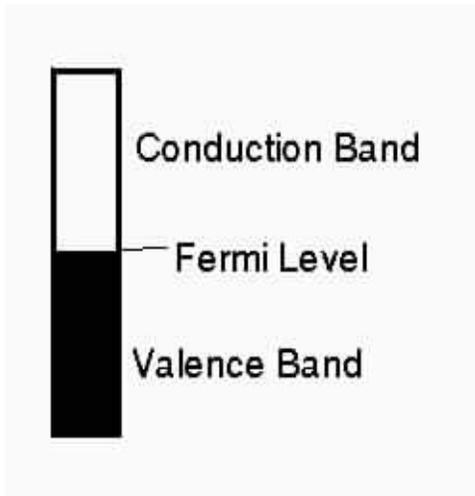
In the above image, the origin of the band becomes quite clear because as the number of molecular orbitals increases, the bonding and antibonding orbitals get closer together filling in the middle. This results in the band seen on the right-hand side. It becomes quite clear that the molecular orbitals become blurred and hence mix with each other, which creates the delocalised cloud of electrons that metals are said to possess.

By describing the molecular orbitals of certain materials as bands, it becomes much easier to understand the properties of [metals](#) and [semi-metals](#). Other materials like [insulators](#) and [semi-conductors](#) will be discussed and concepts such as the [valence band](#), [conduction band](#) and the [Fermi Level](#) will be defined using the band theory



Semi-metal (graphite)





## More on semiconductors

<http://en.wikipedia.org/wiki/Semiconductor>

### Semiconductors

A **semiconductor** is a [solid](#) whose [electrical conductivity](#) is in between that of a [metal](#) and that of an [insulator](#), and can be controlled over a wide range, either permanently or dynamically.<sup>[1]</sup> Semiconductors are tremendously important technologically and economically. [Silicon](#) is the most commercially important semiconductor, though dozens of others are important as well.

[Semiconductor devices](#), electronic components made of semiconductor materials, are essential in modern electrical devices, from [computers](#) to [cellular phones](#) to [digital audio players](#).

#### Overview

Semiconductors are very similar to [insulators](#). The two categories of solids differ primarily in that insulators have larger [band gaps](#) — [energies](#) that [electrons](#) must acquire to be free to flow. In semiconductors at room temperature, just as in insulators, very few

electrons gain enough thermal energy to leap the band gap, which is necessary for [conduction](#). For this reason, pure semiconductors and insulators, in the absence of applied fields, have roughly similar electrical properties. The smaller bandgaps of semiconductors, however, allow for many other means besides [temperature](#) to control their electrical properties.

Semiconductors' [intrinsic](#) electrical properties are very often permanently modified by introducing impurities, in a process known as [doping](#). Usually it is reasonable to approximate that each impurity atom adds one electron or one "hole" (a concept to be discussed later) that may flow freely. Upon the addition of a sufficiently large proportion of dopants, semiconductors conduct [electricity](#) nearly as well as [metals](#). Depending on kind of the impurity, a region of semiconductor can have more electrons or holes, and then it is called [N-type](#) or [P-type](#) semiconductor, respectively. [Junctions between regions of N- and P-type semiconductors](#) have built-in [electric fields](#), which cause electrons and holes to escape from them, and are critical to [semiconductor device](#) operation. Also, a density difference of impurities produces in the region small electric field which is used to accelerate non-equilibrium electrons or holes in it.

In addition to permanent modification through doping, the electrical properties of semiconductors are often dynamically modified by applying [electric fields](#). The ability to control conductivity in small and well-defined regions of semiconductor material, both statically through doping and dynamically through the application of electric fields, has led to the development of a broad range of semiconductor devices, like [transistors](#). Semiconductor devices with dynamically controlled conductivity are the building blocks of [integrated circuits](#), like the [microprocessor](#). These "active" semiconductor devices are combined with simpler [passive components](#), such as semiconductor [capacitors](#) and [resistors](#), to produce a variety of electronic devices.

In certain semiconductors, when electrons fall from the conduction band to the valence band (the energy levels above and below the [band gap](#)), they often emit [light](#). This [photoemission](#) process underlies the [light-emitting diode](#) (LED) and the [semiconductor laser](#), both of which are very important commercially. Conversely, semiconductor absorption of light in [photodetectors](#) excites electrons from the valence band to the conduction band, facilitating reception of [fiber optic communications](#), and providing the basis for [energy](#) from [solar cells](#).

Semiconductors may be elemental materials such as [silicon](#) and [germanium](#), or [compound semiconductors](#) such as [gallium arsenide](#) and [indium phosphide](#), or alloys such as [silicon germanium](#) or [aluminium gallium arsenide](#).

## Band structure



Band structure of a semiconductor showing a full valence band and an empty conduction band.

For more details on this topic, see [Electronic band structure](#).

Like other solids, the electrons in semiconductors can have energies only within certain bands between the energy of the ground state, corresponding to electrons tightly bound to the atomic nuclei of the material, and the free electron energy, which is the energy required for an electron to escape entirely from the material. The energy bands each correspond to a large number of discrete [quantum states](#) of the electrons, and most of the states with low energy are full, up to a particular band called the [valence band](#). Semiconductors and insulators are distinguished from [metals](#) because the valence band in the former materials is very nearly full under normal conditions.

The ease with which electrons in a semiconductor can be excited from the valence band to the conduction band depends on the [band gap](#) between the bands, and it is the size of this energy bandgap that serves as an arbitrary dividing line (roughly 4 [eV](#)) between semiconductors and [insulators](#).

The electrons must move between states to conduct electric current, and so due to the [Pauli exclusion principle](#) full bands do not contribute to the [electrical conductivity](#). However, as the temperature of a semiconductor rises above [absolute zero](#), the states of the electrons are increasingly randomized, or smeared out, and some electrons are likely to be found in states of the [conduction band](#), which is the band immediately above the valence band. The current-carrying electrons in the conduction band are known as "free electrons", although they are often simply called "electrons" if context allows this usage to be clear.

Electrons excited to the conduction band also leave behind [electron holes](#), or unoccupied states in the valence band. Both the conduction band electrons and the valence band holes contribute to electrical conductivity. The holes themselves don't actually move, but a neighbouring electron can move to fill the hole, leaving a hole at the place it has just come from, and in this way the holes appear to move, and the holes behave as if they were actual positively charged particles.

One [covalent bond](#) between neighboring atoms in the solid is ten times stronger than the binding of the single electron to the atom, so freeing the electron does not imply to destroy the crystal structure.

The notion of [holes](#), which was introduced for semiconductors, can also be applied to [metals](#), where the [Fermi level](#) lies *within* the conduction band. **With most metals the [Hall effect](#) reveals electrons to be the charge carriers, but some metals have a mostly filled conduction band, and the [Hall effect](#) reveals positive charge carriers, which are not the ion-cores, but holes.** Contrast this to some [conductors](#) like solutions of [salts](#), or plasma. In the case of a metal, only a small amount of energy is needed for the electrons to find other unoccupied states to move into, and hence for current to flow. Sometimes even in this case it may be said that a hole was left behind, to explain why the electron does not fall back to lower energies: It cannot find a hole. In the end in both materials electron-phonon scattering and defects are the dominant causes for [resistance](#).

The energy distribution of the electrons determines which of the states are filled and which are empty. This distribution is described by [Fermi-Dirac statistics](#). The distribution is characterized by the [temperature](#) of the electrons, and the [Fermi energy](#) or *Fermi level*. Under absolute zero conditions the Fermi energy can be thought of as the energy up to which available electron states are occupied. At higher temperatures, the Fermi energy is the energy at which the probability of a state being occupied has fallen to 0.5.

The dependence of the electron energy distribution on temperature also explains why the conductivity of a semiconductor has a strong temperature dependency, as a semiconductor operating at lower temperatures will have fewer available free electrons and holes able to do the work.

### ***Carrier generation and recombination***

*For more details on this topic, see [Carrier generation and recombination](#).*

When [ionizing radiation](#) strikes a semiconductor, it may excite an electron out of its energy level and consequently leave a hole. This process is known as [electron-hole pair generation](#). Electron-hole pairs are constantly generated from [thermal energy](#) as well, in the absence of any external energy source.

Electron-hole pairs are also apt to recombine. [Conservation of energy](#) demands that these recombination events, in which an electron loses an amount of [energy](#) larger than the

[band gap](#), be accompanied by the emission of thermal energy (in the form of [phonons](#)) or radiation (in the form of [photons](#)).

In the steady state, the generation and recombination of electron–hole pairs are in equipoise. The number of electron-hole pairs in the [steady state](#) at a given temperature is determined by [quantum statistical mechanics](#). The precise [quantum mechanical](#) mechanisms of generation and recombination are governed by [conservation of energy](#) and [conservation of momentum](#).

As probability that electrons and holes meet together is proportional to the product of their amounts, the product is in steady state nearly constant at a given temperature, providing that there is no significant electric field (which might "flush" carriers of both types, or move them from neighbour regions containing more of them to meet together) or externally driven pair generation. The product is a function of the temperature, as the probability of getting enough thermal energy to produce a pair increases with temperature, being approximately  $1/\exp(\text{band gap} / kT)$ , where  $k$  is [Boltzmann's constant](#) and  $T$  is absolute temperature.

The probability of meeting is increased by carrier traps – impurities or dislocations which can trap an electron or hole and hold it until a pair is completed. Such carrier traps are sometimes purposely added to reduce the time needed to reach the steady state.

## **Doping**

*For more details on this topic, see [Doping \(semiconductor\)](#).*

The property of semiconductors that makes them most useful for constructing electronic devices is that their conductivity may easily be modified by introducing impurities into their [crystal lattice](#). The process of adding controlled impurities to a semiconductor is known as *doping*. The amount of impurity, or dopant, added to an [intrinsic](#) (pure) semiconductor varies its level of conductivity. Doped semiconductors are often referred to as [extrinsic](#).

## **Dopants**

The materials chosen as suitable dopants depend on the atomic properties of both the dopant and the material to be doped. In general, dopants that produce the desired controlled changes are classified as either electron acceptors or donors. A donor atom that activates (that is, becomes incorporated into the crystal lattice) donates weakly-bound valence electrons to the material, creating excess negative [charge carriers](#). These weakly-bound electrons can move about in the crystal lattice relatively freely and can facilitate conduction in the presence of an electric field. (The donor atoms introduce some states under, but very close to the conduction band edge. Electrons at these states can be easily excited to conduction band, becoming free electrons, at room temperature.) Conversely, an activated acceptor produces a hole. Semiconductors doped with donor impurities are called *n-type*, while those doped with acceptor impurities are known as *p-type*. The n and p type designations indicate which charge carrier acts as the material's [majority carrier](#).

The opposite carrier is called the [minority carrier](#), which exists due to thermal excitation at a much lower concentration compared to the majority carrier.

For example, the pure semiconductor [silicon](#) has four valence electrons. In silicon, the most common dopants are [IUPAC group 13](#) (commonly known as *group III*) and [group 15](#) (commonly known as *group V*) elements. Group 13 elements all contain three valence electrons, causing them to function as acceptors when used to dope silicon. Group 15 elements have five valence electrons, which allows them to act as a donor. Therefore, a silicon crystal doped with [boron](#) creates a p-type semiconductor whereas one doped with [phosphorus](#) results in an n-type material.

## Carrier concentration

The concentration of dopant introduced to an intrinsic semiconductor determines its concentration and indirectly affects many of its electrical properties. The most important factor that doping directly affects is the material's carrier concentration. In an intrinsic semiconductor under thermal equilibrium, the concentration of electrons and holes is equivalent. That is,

$$n = p = n_i$$

Where  $n$  is the concentration of conducting electrons,  $p$  is the electron hole concentration, and  $n_i$  is the material's intrinsic carrier concentration. Intrinsic carrier concentration varies between materials and is dependent on temperature. Silicon's  $n_i$ , for example, is roughly  $1 \times 10^{10} \text{ cm}^{-3}$  at 300 [kelvins](#) (room temperature).

In general, an increase in doping concentration affords an increase in conductivity due to the higher concentration of carriers available for conduction. Degenerately (very highly) doped semiconductors have conductivity levels comparable to metals and are often used in modern [integrated circuits](#) as a replacement for metal. Often superscript plus and minus symbols are used to denote relative doping concentration in semiconductors. For example,  $n^+$  denotes an n-type semiconductor with a high, often degenerate, doping concentration. Similarly,  $p^-$  would indicate a very lightly doped p-type material. It is useful to note that even degenerate levels of doping imply low concentrations of impurities with respect to the base semiconductor. In crystalline intrinsic silicon, there are approximately  $5 \times 10^{22} \text{ atoms/cm}^3$ . Doping concentration for silicon semiconductors may range anywhere from  $10^{13} \text{ cm}^{-3}$  to  $10^{18} \text{ cm}^{-3}$ . Doping concentration above about  $10^{18} \text{ cm}^{-3}$  is considered degenerate at room temperature. Degenerately doped silicon contains a proportion of impurity to silicon in the order of parts per thousand. This proportion may be reduced to parts per billion in very lightly doped silicon. Typical concentration values fall somewhere in this range and are tailored to produce the desired properties in the device that the semiconductor is intended for.

## Effect on band structure



[Band diagram](#) of a  $p^+n$  junction. The band bending is a result of the positioning of the Fermi levels in the  $p^+$  and  $n$  sides.

Doping a semiconductor crystal introduces allowed energy states within the band gap but very close to the energy band that corresponds with the dopant type. In other words, donor impurities create states near the conduction band while acceptors create states near the valence band. The gap between these energy states and the nearest energy band is usually referred to as dopant-site bonding energy or  $E_B$  and is relatively small. For example, the  $E_B$  for [boron](#) in silicon bulk is 0.045 eV, compared with silicon's band gap of about 1.12 eV. Because  $E_B$  is so small, it takes little energy to ionize the dopant atoms and create free carriers in the conduction or valence bands. Usually the thermal energy available at room temperature is sufficient to ionize most of the dopant.

Dopants also have the important effect of shifting the material's Fermi level towards the energy band that corresponds with the dopant with the greatest concentration. Since the Fermi level must remain constant in a system in [thermodynamic equilibrium](#), stacking layers of materials with different properties leads to many useful electrical properties. For example, the [p-n junction's](#) properties are due to the energy band bending that happens as a result of lining up the Fermi levels in contacting regions of p-type and n-type material.

This effect is shown in a [band diagram](#). The band diagram typically indicates the variation in the valence band and conduction band edges versus some spatial dimension, often denoted  $x$ . The Fermi energy is also usually indicated in the diagram. Sometimes the *intrinsic Fermi energy*,  $E_i$ , which is the Fermi level in the absence of doping, is shown. [These diagrams are useful in explaining the operation of many kinds of semiconductor devices.](#)

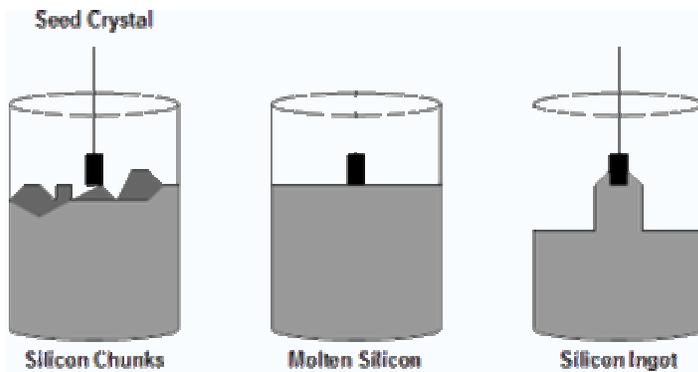
## ***Preparation of semiconductor materials***

Semiconductors with predictable, reliable electronic properties are necessary for [mass production](#). The level of chemical purity needed is extremely high because the presence of impurities even in very small proportions can have large effects on the properties of the material. A high degree of crystalline perfection is also required, since faults in crystal structure (such as [dislocations](#), [twins](#), and [stacking faults](#)) interfere with the semiconducting properties of the material. Crystalline faults are a major cause of defective semiconductor devices. The larger the crystal, the more difficult it is to achieve the necessary perfection. Current mass production processes use crystal [ingots](#) between four and twelve inches (300 mm) in diameter which are grown as cylinders and sliced into [wafers](#).

Because of the required level of chemical purity and the perfection of the crystal structure which are needed to make semiconductor devices, special methods have been developed to produce the initial semiconductor material. A technique for achieving high purity includes growing the crystal using the [Czochralski process](#). An additional step that can be used to further increase purity is known as [zone refining](#). In zone refining, part of a solid crystal is melted. The impurities tend to concentrate in the melted region, while the desired material recrystallizes leaving the solid material more pure and with fewer crystalline faults.

In manufacturing semiconductor devices involving [heterojunctions](#) between different semiconductor materials, the [lattice constant](#), which is the length of the repeating element of the crystal structure, is important for determining the compatibility of materials.

## **Czochralski process**



 The Czochralski process

The **Czochralski process** is a method of [crystal](#) growth used to obtain [single crystals](#) of [semiconductors](#) (e.g. [silicon](#), [germanium](#) and [gallium arsenide](#)), metals (e.g. [palladium](#), [platinum](#), [silver](#), [gold](#)), salts and some man made, (or "lab") [gemstones](#).

The most important application may be the growth of large cylindrical [ingots](#), or [boules](#), of [single crystal silicon](#). High-purity, [semiconductor-grade](#) silicon (only a few parts per million of impurities) is melted down in a [crucible](#), which is usually made of [quartz](#). Dopant impurity atoms such as [boron](#) or [phosphorus](#) can be added to the molten intrinsic silicon in precise amounts in order to dope the silicon, thus changing it into n-type or p-type extrinsic silicon. This influences the [electrical conductivity](#) of the silicon. A [seed crystal](#), mounted on a rod, is dipped into the molten silicon. The seed crystal's rod is pulled upwards and rotated at the same time. By precisely controlling the temperature gradients, rate of pulling and speed of rotation, it is possible to extract a large, single-crystal, cylindrical ingot from the melt. This process is normally performed in an [inert](#) atmosphere, such as [argon](#), and in an inert chamber, such as [quartz](#).

While the largest silicon ingots produced today are 400 [mm](#) in diameter and 1 to 2 [metres](#) in length, 200 mm and 300 mm diameter crystals are standard industrial processes. Thin silicon [wafers](#) are cut from these ingots (typically about 0.75 mm thick) and polished to a very high flatness to be used for creating [integrated circuits](#). Other semiconductors, such as [gallium arsenide](#), can also be grown by this method, although lower defect densities in this case can be obtained using variants of the [Bridgeman technique](#).

When silicon is grown by the Czochralski method the melt is contained in a [silica](#) ([quartz](#)) crucible. During growth the walls of the crucible dissolve into the melt and Czochralski silicon therefore contains [oxygen](#) impurities with a typical concentration of  $10^{18} \text{cm}^{-3}$ . Perhaps surprisingly, oxygen impurities can have beneficial effects. Carefully chosen annealing conditions can allow the formation of oxygen [precipitates](#). These have the effect of trapping unwanted [transition metal](#) impurities in a process known as [gettering](#). Additionally, oxygen impurities can improve the mechanical strength of silicon wafers by immobilising any [dislocations](#) which may be introduced during device processing. It has experimentally been proved in the 1990s that the high oxygen concentration is also beneficial for [radiation hardness](#) of silicon [particle detectors](#) used in harsh radiation environment ( e.g. [CERN's LHC/S-LHC projects](#))<sup>[1][2][3]</sup> Therefore,

radiation detectors made of Czochralski- and Magnetic Czochralski-silicon are considered to be promising candidates for many future high-energy physics experiments. <sup>[4][5]</sup>

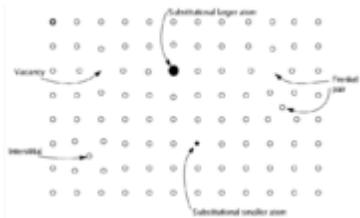
## Crystal Imperfections:

Important as order is.

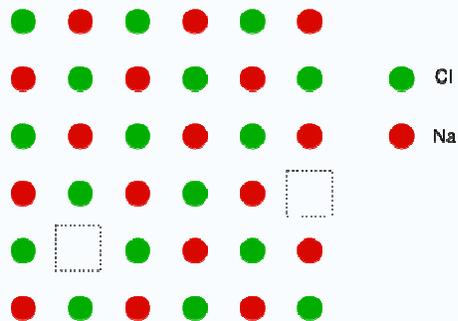
Imperfections reflect entropy

### I. Point Defects:

- a) Frenkel defects: Creation of a vacancy by removal to an interstitial position.
- b) Schottky defects: In ionic crystals, vacancy formation occurs in such a way to maintain electrical neutrality.



Schematic illustration of some simple point defect types in a monatomic solid



Schematic Schottky defects.

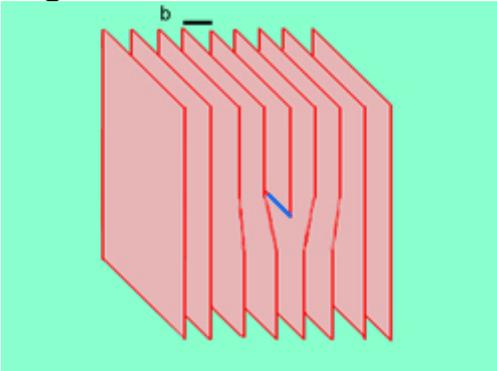
### II. Line Defects (Dislocations):

Occur during crystal growth. Two types:

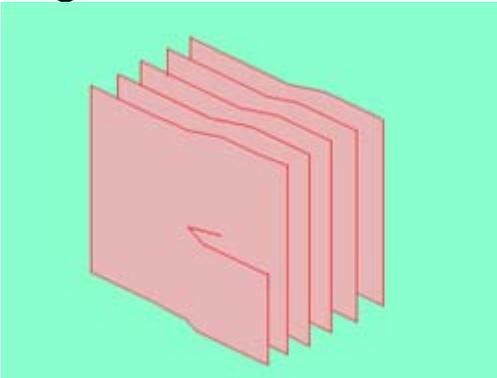
- a) Screw-Dislocation

b) Edge-Dislocation

Figures here



Edge-Dislocation

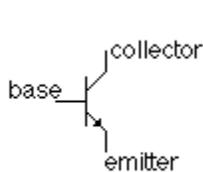


Screw Dislocation



# The transistor:

- <http://www.physlink.com/Education/AskExperts/ae430.cfm>
- 
- How does a transistor work?
- Answer



Typical transistor packages

- 
- 

**The design of a transistor allows it to function as an amplifier or a switch.** This is accomplished by using a small amount of electricity to control a gate on a much **larger supply of electricity**, much like turning a valve to control a supply of water.

- Transistors are composed of three parts – a **base**, a **collector**, and an **emitter**.
- **The base is the gate controller device for the larger electrical supply.**
- **The collector is the larger electrical supply,**
- and the **emitter is the outlet for that supply.**
- By sending varying levels of current from the base, **the amount of current flowing through the gate from the collector may be regulated.**
- In this way, a very small amount of current may be used to control a large amount of current, as in an amplifier.
- **The same process is used to create the binary code for the digital processors but in this case a voltage threshold of five volts is needed to open the collector gate. In this way, the transistor is being used as a switch with a binary function: five volts – ON, less than five volts – OFF.**

Semi-conductive materials are what make the transistor possible. Most people are familiar with electrically conductive and non-conductive materials. Metals are typically thought of as being conductive. Materials such as wood, plastics, glass and ceramics are non-conductive, or insulators. In the late 1940's a team of scientists working at Bell Labs in New Jersey, discovered how to take certain types of crystals and use them as electronic control devices by exploiting their semi-conductive properties. Most non-metallic crystalline structures would typically be

considered insulators. But by forcing crystals of germanium or silicon to grow with impurities such as boron or phosphorus, the crystals gain entirely different electrical conductive properties. **By sandwiching this material between two conductive plates (the emitter and the collector), a transistor is made.** By applying current to the semi-conductive material (base), electrons gather until an effectual conduit is formed allowing electricity to pass. The scientists that were responsible for the invention of the transistor were John Bardeen, Walter Brattain, and William Shockley. Their Patent was called: "Three Electrode Circuit Element Utilizing Semiconductive Materials."

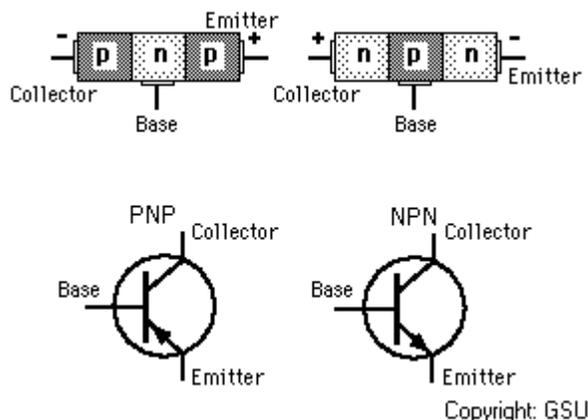
Answered by: Stephen Portz, Technology Teacher, Space Coast Middle School, FL

**There are two main types of transistors: junction transistors and field effect transistors.** Each works in a different way. **But the usefulness of any transistor comes from its ability to control a strong current with a weak voltage.** For example, transistors in a public address system amplify (strengthen) the weak voltage produced when a person speaks into a microphone. The electricity coming from the transistors is strong enough to operate a loudspeaker, which produces sounds much louder than the person's voice.

## JUNCTION TRANSISTORS

A junction transistor consists of a thin piece of one type of semiconductor material between two thicker layers of the opposite type. For example, if the middle layer is p-type, the outside layers must be n-type. **Such a transistor is an NPN transistor. One of the outside layers is called the emitter, and the other is known as the collector.** The middle layer is the base. The places where the emitter joins the base and the base joins the collector are called junctions.

**The layers of an NPN transistor must have the proper voltage connected across them. The voltage of the base must be more positive than that of the emitter. The voltage of the collector, in turn, must be more positive than that of the base. The voltages are supplied by a battery or some other source of direct current (DC). The emitter supplies electrons. The base pulls these electrons from the emitter because it has a more positive voltage than does the emitter. This movement of electrons creates a flow of electricity through the transistor.**



The current passes from the emitter to the collector through the base. Changes in the voltage connected to the base modify the flow of the current by changing the number of electrons in the base. In this way, small changes in the base voltage can cause large changes in the current flowing out of the collector.

Manufacturers also make PNP junction transistors. In these devices, the emitter and collector are both a p-type semiconductor material and the base is n-type. A PNP junction transistor works on the same principle as an NPN transistor. But it differs in one respect. The main flow of current in a PNP transistor is controlled by altering the number of holes rather than the number of electrons in the base. Also, this type of transistor works properly only if the negative and positive connections to it are the reverse of those of the NPN transistor. Base must have less positive (more negative) potential than emitter.

## FIELD EFFECT TRANSISTORS (FET)

A field effect transistor (FET) has only two layers of semiconductor material, one on top of the other. Electricity flows through one of the layers, called the channel. A voltage connected to the other layer, called the gate, interferes with the current flowing in the channel. Thus, the voltage connected to the gate controls the strength of the current in the channel.

There are two basic types of field effect transistors-

- junction field effect transistor (JFET) and
- metal oxide semiconductor field effect transistor (MOSFET). Most of the transistors contained in today's integrated circuits are MOSFETS's.

