Atomic Theory

It is necessary to know what goes on at the atomic level of a semiconductor so the characteristics of the semiconductor can be understood. In many cases a detailed explanation of why some of the phenomena occur is not required or supplied. Just knowing that certain phenomena do occur allows us to understand why semiconductors behave the way they do.

The Atom

Figure 1 shows a representation of the Bohr atom. The atom contains three basic particles; ***protons*** and ***neutrons*** that make up the ***nucleus*** of the atom and ***electrons*** that orbit the nucleus.

- The ***protons*** have a ***one positive charge*** and have ***significant mass***
- The ***neutrons*** have ***no charge*** but essentially the ***same mass*** as protons
- The ***electrons*** have ***one negative charge*** and have ***negligible mass.***
- ***Protons & neutrons*** form the nucleus of an atom.
- Electrons orbit the nucleus in ***orbitals*** or ***shells***.

Normally the number of electrons orbiting the nucleus equals the number of protons in the nucleus. This means the atom is electrically neutral; the number of negative charges equals the number of positive charges. Electrons travel in orbital shells. They normally remain in these shells unless they are stimulated by some external energy source.

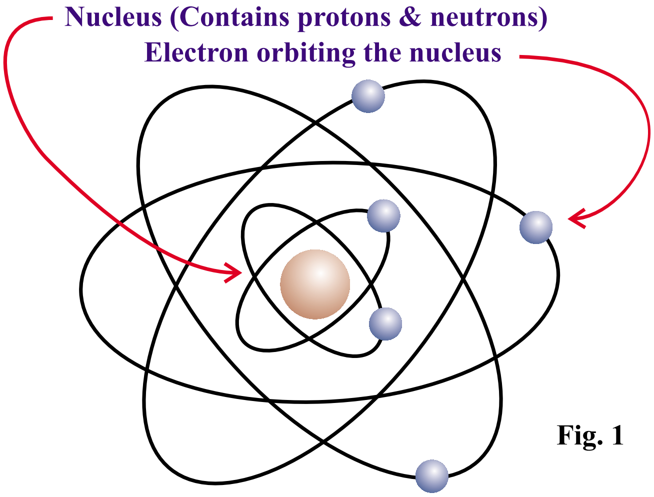
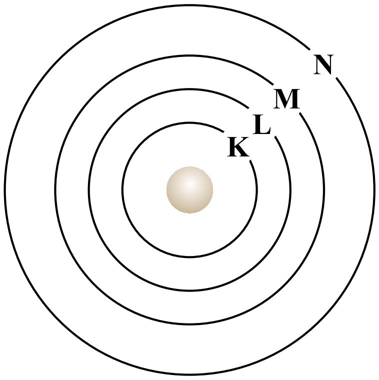


Fig. 1

The Bohr Model



Shells or Energy Levels

Figure 2

The orbital paths or shells are identified using letters K through Q. The inner most shell is the K shell, followed by the L shell. The other shells are labelled as shown in Figure 2. The outer most shell for a given atom is called the valence shell. The valence shell is important because it determines the conductivity of the atom. The valence shell of atom can contain up to eight ***valence electrons***. The conductivity of the atom depends on the number of electrons that are in the valence shell. When an atom has only one electron in valence shell, it is almost a perfect conductor. When an atom has eight valence electrons the valence shell is said to be complete and the atom is an insulator. The conductivity of an element decreases as the number of electrons in the valence shells are increased.

Conductors

A conductor is a material that allows electrons to easily pass through it. Copper is a good conductor. Note that the valence shell has only one electron.

With atoms:

- K is full with 2 electrons
- L is full with 8 electrons
- M is full with 18 electrons

This totals 28 electrons with 1 electron left in the N shell (valence shell for copper)

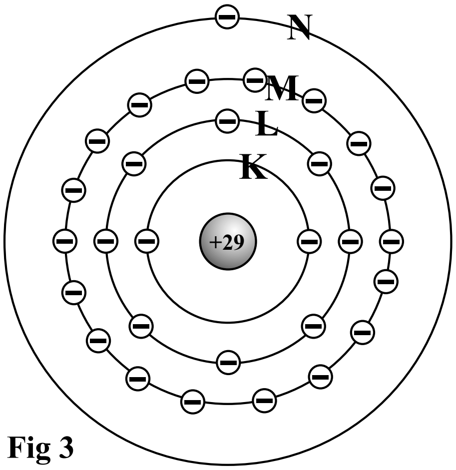


Fig 3

Copper Atom
29 protons
29 electrons
35 neutrons

The valence shell ideally needs 8 electrons to be full but copper has only one. The energy required to allow this electron to escape the valence shell and become free depends on the number of electrons in the valence shell. Since there is only one here, freedom is easy. A slight voltage force will free it. Even the heat at room temperature will free some of them.

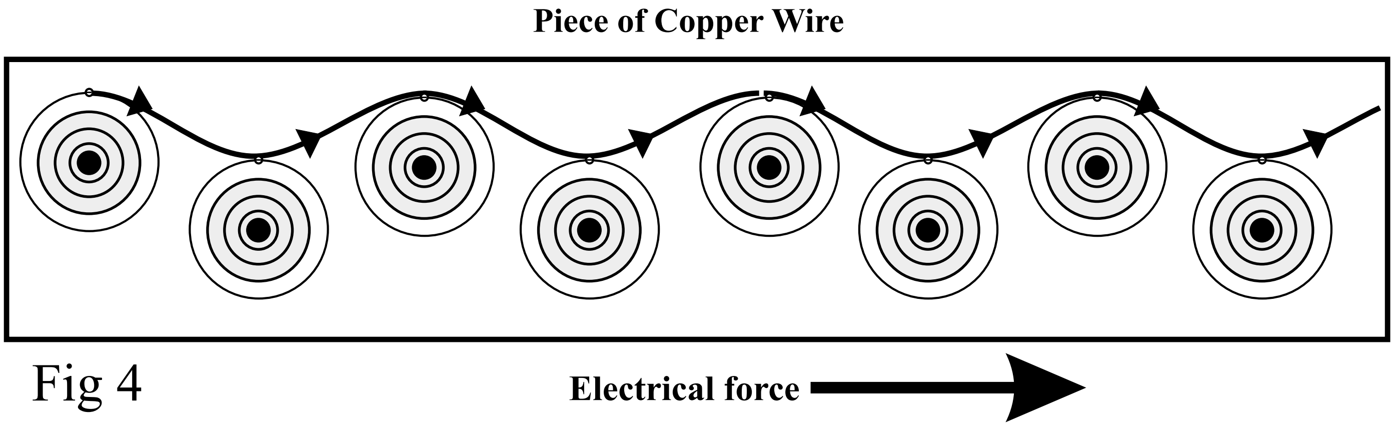


Fig 4

Application of a the slightest electrical force will cause these electrons to move from atom to atom down the wire.

The best conductors are Silver , Copper & Gold. ***All have one valence electron.***

Semiconductors

Semiconductors are atoms that contain 4 valence electrons.

Remember that a good conductor has 1 valence electrons and an insulator has eight valence electrons.

The semiconductor has 4 valence electrons. It is neither a good conductor or a good insulator.

Three of the most commonly used semiconductor materials are silicon (Si), germanium (Ge), and carbon (C). These atoms are shown Figure 5.. Note that all of them have 4 valence electrons.

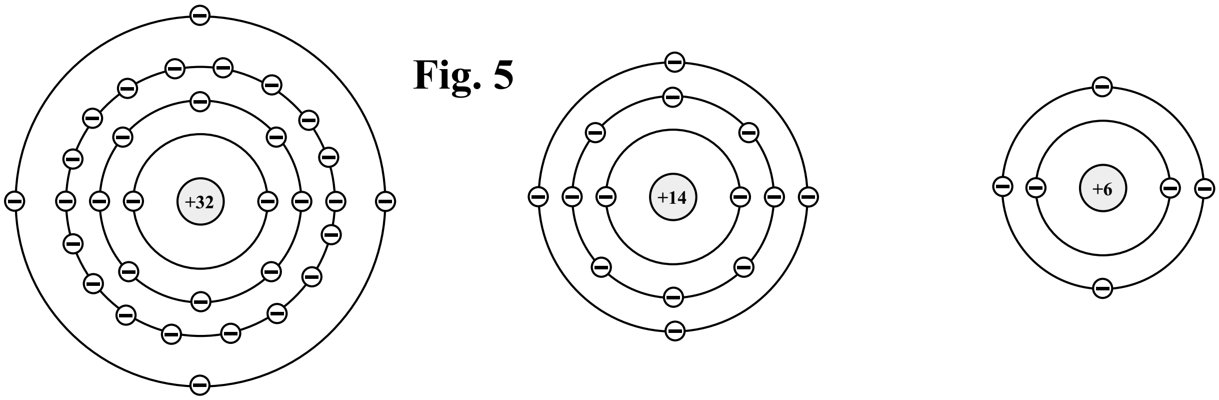


Fig. 5

Germanium Atom   Silicon Atom   Carbon Atom

Ions

When the number of protons in an atom equals the number of electrons the atom is said to be neutral. When no outside force causes conduction, the atom will remain neutral.

If an atom loses one valence electron, then the net charge on the atom is positive. The atom is now have positive ion.

If an atom with an incomplete valence shell gains one valence electron, then the atom would be negative. This is because there would be one extra electron in the atom.

In summary, if the atom has more electrons then protons, it will have a negative charge and become a negative ion. If the atom has more protons that electrons it will have a positive charge and become a positive ion.

Charge and Conduction

Some fundamentalrules regarding the relationship between electrons and orbital shells have been shown the be true. They are listed below:

1) *Electrons travel in an orbital shell. They cannot orbit the nucleus in the space that exists between any two orbital shells.*

2) *Each orbital shell relates to a specific energy range. Thus, all the electrons travelling in a given orbital shell will contain the same relative amount of energy.*

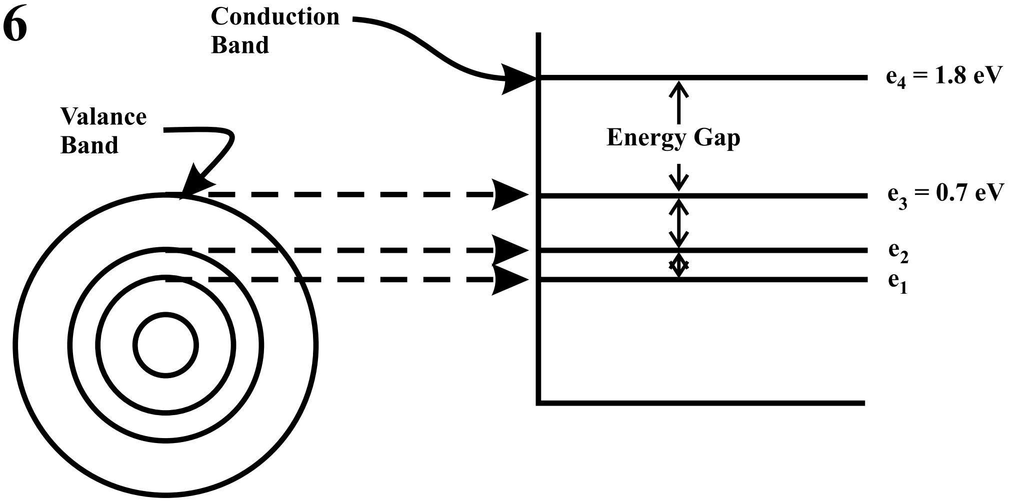
Note that the energy levels for a given shell increase as you move away from the nucleus. Thus, the valence electrons will always have the highest energy levels in a given atom.

3) *For an electron to jump from one shell to another, it must absorb enough energy to make up the difference between its initial energy level, and the energy level of the shell to which it is jumping.*

4) *If an electron absorbs enough energy, to jump from one shell to another, it will eventually give up the energy it absorbed and return to a lower energy shell.*

Silicon Energy Gaps and Levels

Fig. 6



Charge and Conduction

Examine Figure 6. The space between any two orbital shells is referred to as an energy gap. Electrons travel through the energy gap when going from one shell to another, but they cannot continually orbit the nucleus of the atom in one of the energy gaps.

Each orbital shell is related to a specific energy level. For an electron to jump from one orbital shell to another, it must absorb enough energy to make up the difference between the shells.

For example in Figure 6, the valence shell, or band, is shown to have an energy level of approximately 0.7 electron volt (eV). The conduction band is shown to have an energy level of 1.8 eV. For an electron to jump from the valence band to the conduction band, it would have to absorb an amount of energy equal to:

$$1.8 \text{ eV} - 0.7 \text{ eV} = 1.1 \text{ eV}$$

For conductors, semiconductors, and insulators, the valence to conduction band energy gaps are approximately 0.4, 1.1, and 1.8 electron volts respectively. The higher the energy gap, the harder it is to have conduction because more energy must be absorbed for an electron to jump to the conduction band.

When an electron absorbs enough energy to jump from the valence band to the conduction band, the electron is said to be in an ***excited state.*** An excited electron will eventually give up the energy it absorbed and return to its original energy level. The energy given up by the electron is in the form of light or heat.

Covalent Bonding

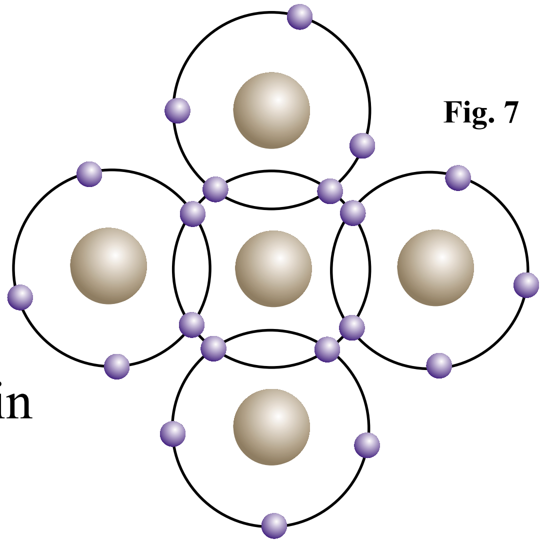


Fig. 7

Silicon Covalent Bonding

Covalent bonding is a method by which atoms complete their valence shells by sharing valence electrons with other atoms.

Figure 7 shows 5 silicon atoms that are in a covalent bond. We know that each silicon atoms has 4 valence electrons in the outer shell.

Note that the silicon atom in the centre of the group has 8 electrons in its valence shell. It is sharing one electron from each of the surrounding 4 silicon atoms to complete its valence shell.

This process is carried on over and over again with each silicon atom sharing electrons with its neighbour. In this way all of the silicon atoms have 8 electrons in their valence shell, except the atoms on the very edge of the crystal. These atoms remain with incomplete valence shells.

The results of covalent bonding are:

- The atoms are held together forming a solid substance(in this case, a crystal)
- The atoms are electrically stable because their valence shells are complete.

Heat Energy and Holes

If the silicon crystal is pure, all of the valence shells will be complete. There will be no free electrons available in the crystal.

This will make pure silicon a poor conductor of electrons. Pure silicon is called ***intrinsic.*** Intrinsic is simply another way of saying pure. Intrinsic Germanium is also a poor conductor of electrons.

When semiconductor atoms bond together in a set pattern like the one shown in Figure 7, the resulting material is called a crystal. A crystal is a smooth glass like solid. Both Silicon and Germanium crystallize in the same fashion.

Heat energy and holes

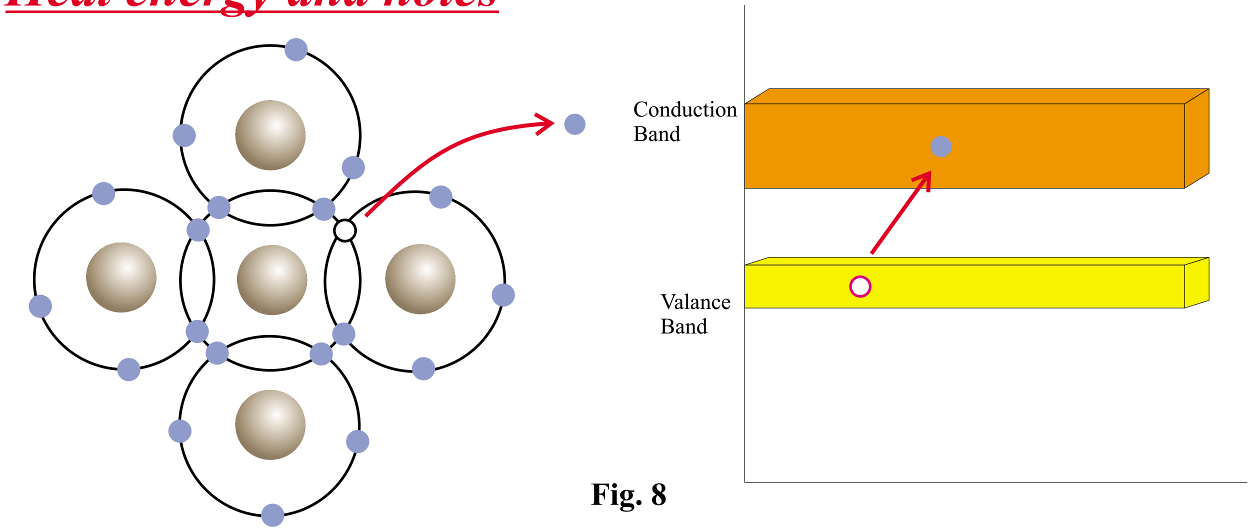


Fig. 8

Generation of an electron-hole pair

Heat energy causes the atoms in material to vibrate. If you pick up a warm object, the warmth that you feel is caused by the vibrating atoms.

The higher the ambient temperature, the stronger the mechanical vibration will be. These vibrations can occasionally dislodge an electron from the valence orbit.

When this happens, the electron will move to the conduction band (See Figure 8). It is now a free electron and it can move about the crystal.

When an electron leaves the valence orbit, it leaves behind a vacancy. This vacancy is called a hole. This hole behaves like a positive charge because it will attract and hold any free electron close to it.

In an intrinsic silicon crystal, ***equal numbers of free electrons and holes are created by heat energy***. If the free electron in the conduction band passes close to a hole, it will give up its energy and drop back into the hole.

This process use called ***re-combination***. The time between an electron jumping into the conduction band (becoming to free electron) and re-combination is called the ***lifetime*** of the electron hole pair. This lifetime is generally very short (only a few S).

At room temperature, the following is taking place inside the crystal.

- **Some free electrons and holes are being created by thermal energy.**
- **Other free electrons and holes are re-combining.**
- **Some are in an in-between state.**

At absolute zero (-273^{O}C) there are no electron-hole pairs being created so there are no free electrons. The number of hole pairs increases proportionately with an increase in temperature. This means that the number of free electrons available increases as the temperature of the crystal rises.

Holes and the Intrinsic Semi-Conductor

A silicon crystal is an intrinsic semiconductor if every atom is a silicon atom. At room temperature -- silicon acts as almost an insulator because room temperature thermal energy creates only a few electron-hole pairs.

A very small current can be created by using the circuit shown in Figure 9. The diagram shows a pure silicon crystal at room temperature that is between two charged metal plates.

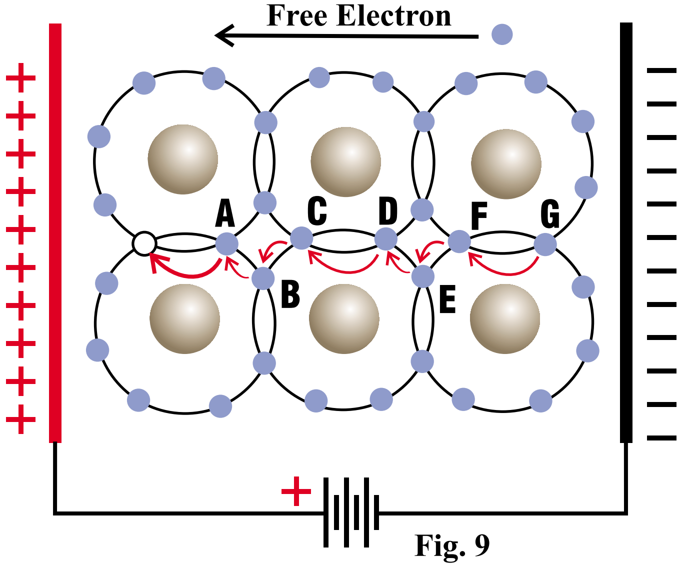


Fig. 9
Current Flow in an Intrinsic Crystal
The Flow of Holes

Assume that thermal energy has produced one electron-hole pair. The free electron is in the conduction band at the right end of the crystal.

We will use electron flow to explain how the current flows.

The negative plate will repel the free electron to the left in the direction of the arrow. The electron will travel in the conduction band, from atom to atom, until it reaches the right plate and leaves the crystal.

For every electron that leaves the crystal via the positive plate, one electron must enter the crystal via the negative plate. In order for this to take place - the following will happen.

The Flow of Holes

Look at Figure 9 again. Notice the hole at the left.

The hole attracts the valence electron at point “A”. The valence electron moves from “A” and fills the hole. Now a hole exists at “A”

The hole now at “A” attracts the valence electron at point “B”
The electron at “B” moves into the hole making a new hole at “B”

The hole now at “B” attracts the valence electron at point “C”
The electron at “C” moves into the hole making a new hole at “C”

The process continues from “C” to “G” until the hole is close to the negative plate.

Now an electron from the negative plate falls into the hole. The circuit has now been completed.

If we imagine all of these actions happening quickly, the valence electrons are moving to the left while the holes appear to move to the right along the path A-B-C-D-E-F-G.

Note that we said that valence electrons are moving here. This action is not the same as re-combination where a free electron falls into a hole. The valence electrons do the moving here.

Two Types of Flow

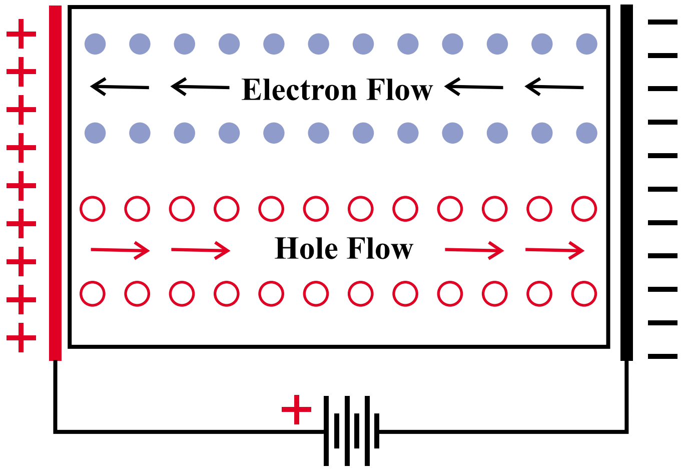
We know that an intrinsic semiconductor has the same number of free electrons and holes because heat produces them in pairs.

In Figure 10, the applied voltage will cause the free electrons to move to the left and the holes to move to the right.

We will visualize the current in a semi-conductor as the combined effect of two types of flow

- ***Free electron flow in one direction***
- ***Flow of holes in the other direction***

These free electrons and holes are called ***carriers*** because they carry a charge from one place to another.



Conduction vs temperature

- **Electrons and holes are in pairs.**
- **Electron hole pairs are caused by heat**
- **At absolute zero - no pairs are created and the current flow is zero.**
- **As the temperature of the crystal rises - the current increases proportionately.**
- **Conductivity in a semiconductor is directly proportional to temperature.**

Fig. 10 **Electron and hole flow in a semiconductor crystal**

Doping

Intrinsic (pure) silicon and germanium are poor conductors. The current flow at room temperature is very small. Because of their poor conductivity, intrinsic silicon and germanium are of little use.

The doping is the process of adding impurity atoms to intrinsic silicon or germanium to improve the conductivity of the semiconductor. The term impurity is used to describe the doping elements. Since the doped semiconductor is no longer pure, it is called an extrinsic semiconductor.

To types of elements are used for doping: trivalent and pentavalent. At trivalent element is one that has three valence electrons. At pentavalent element is one that has five valence electrons.

p-type material is created by adding trivalent atoms to an intrinsic semiconductor.

n-type material is created by adding pentavalent atoms to an intrinsic semiconductor.

The commonly used elements are shown Figure 12.

Commonly Used Doping Elements

Trivalent Impurities	Pentavalent Impurities
Aluminum (Al)	Phosphorus (P)
Gallium (Ga)	Arsenic (As)
Boron (B)	Antimony (Sb)
Indium (In)	Bismuth (Bi)

Figure 12

Increasing Free Electrons - n type material

When pentavalent impurities are added to silicon or germanium, the result is an excess of electrons in the covalent bonds. Figure 13 (a) shows the pentavalent arsenic atom surrounded by four silicon atoms.

The silicon atoms each form covalent bonds with the arsenic atom. The arsenic atom has 5 electrons but only 4 are used in the covalent bonds. The fifth electron can easily break free and enter the conduction band.

If millions of arsenic atoms are added to pure silicon, there will be millions of these electrons that can be made to flow through the material with little difficulty.

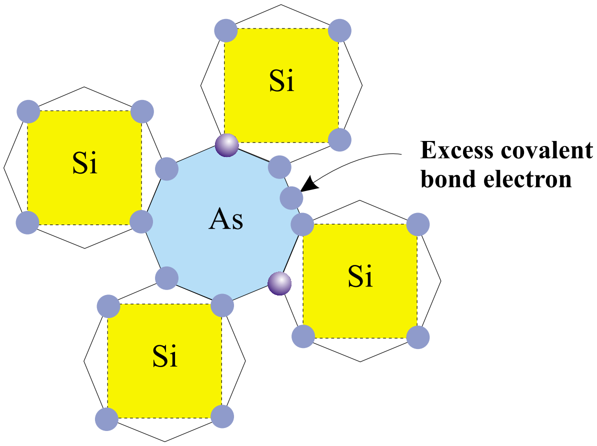


Fig 13 (a)

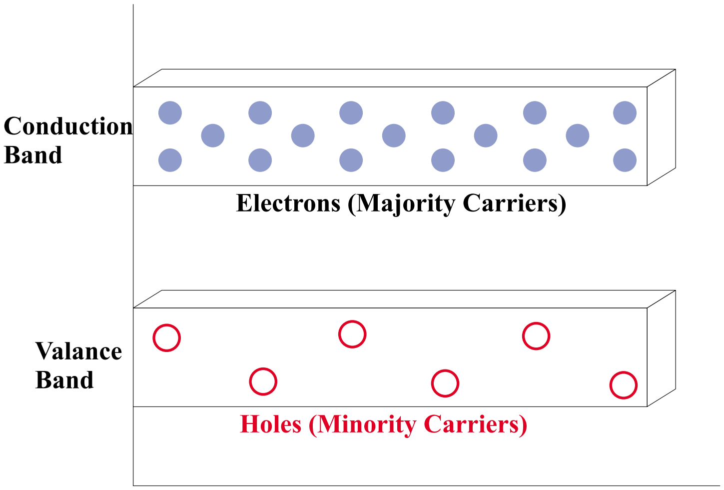


Fig 13 (b)

n- type material with pentavalent impurity

It is important note that even though there are many free electrons in the material now, the crystal is still electrically neutral. This is because the number of protons in the material still equals the number of electrons. The net charge on material is zero.

This n type material contains many more free electrons in the conduction band than holes. The electrons are called majority carriers and the valence band holes are called minority carriers.

Figure 13 (b) shows the relationship between these two types of carriers. The valence band is shown to contain some holes. These holes are caused by thermal energy excitation of electrons as we discussed earlier.

There is an excess of conduction band electrons and any hole that is created by thermal energy is quickly filled by and nearby free electron. This means that the lifetime of an electron-hole pair in shortened significantly.

Since the only holes that exist in the covalent bonding are those caused by thermal energy, the number of holes is far less than the number of conduction band electrons. This is where the term majority and minority comes from.

In n-type material, the ***electrons are the majority carriers*** and the ***holes are the minority carriers.***

It is important to note that even though there are many free electrons, the number of electrons equals the number of protons in the material This is because the free electron was donated by the arsenic atom. Both arsenic and silicon atoms were neutral when they were combined together to form the new material. They remain neutral after they are bonded. The free electron is a result of the covalent bonding. This means all of the free electrons in the conduction band must remain in the material in order for it to be neutral.

The arsenic atom is called that donor atom because it donatesthe free electrons to the material.

Increasing Holes - p type material

When trivalent impurities are added to silicon or germanium, the covalent bonds form with a hole in their structure. If you look at Figure 14(a), you see 4 silicon atoms surrounding an aluminum atom.

Since aluminum has only 3 valence electrons, and each of the 4 silicon atoms wants to share one each, these is a shortage of one electron. This gap or hole is illustrated in Figure 14(a).

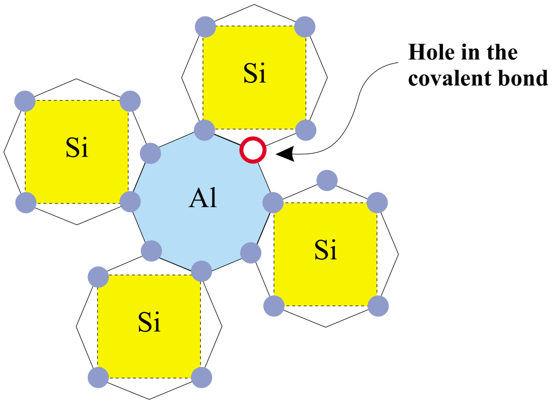


Fig 14 (a)

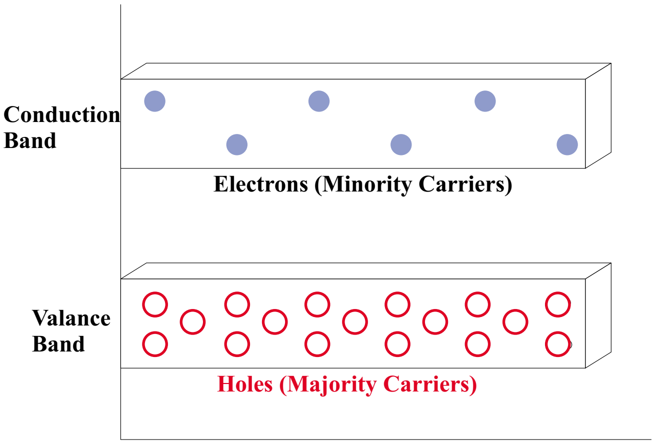


Fig 14 (b)

p- type material with trivalent impurity

Figure 14(b) shows that this time we have an excess of holes in the valence band. At the same time, there are some free electrons in the conduction band. These are caused by thermal energy.

Since there are many more valence band holes than conduction band electrons, the holes are the majority carriers and the electrons are the minority carriers.

Even though there are many holes in the material, the number of electrons equals the number of protons. This is because the hole was created as a result of the covalent bonding between the silicon and the aluminum atoms. Both aluminum and silicon atoms were neutral when they were combined together to form the new material. They remain neutral after they are bonded. This means all of the holes in the valence band must remain empty in the material in order for it to be neutral.

The ***trivalent atoms*** are called ***acceptor atoms***. The reason for this will be explained later.

The pn Junction

Figure 15 shows the initial energy levels of p and n-type materials. The top diagram shows n -type material containing an excess of electrons while the p-type material contains an excess of holes.

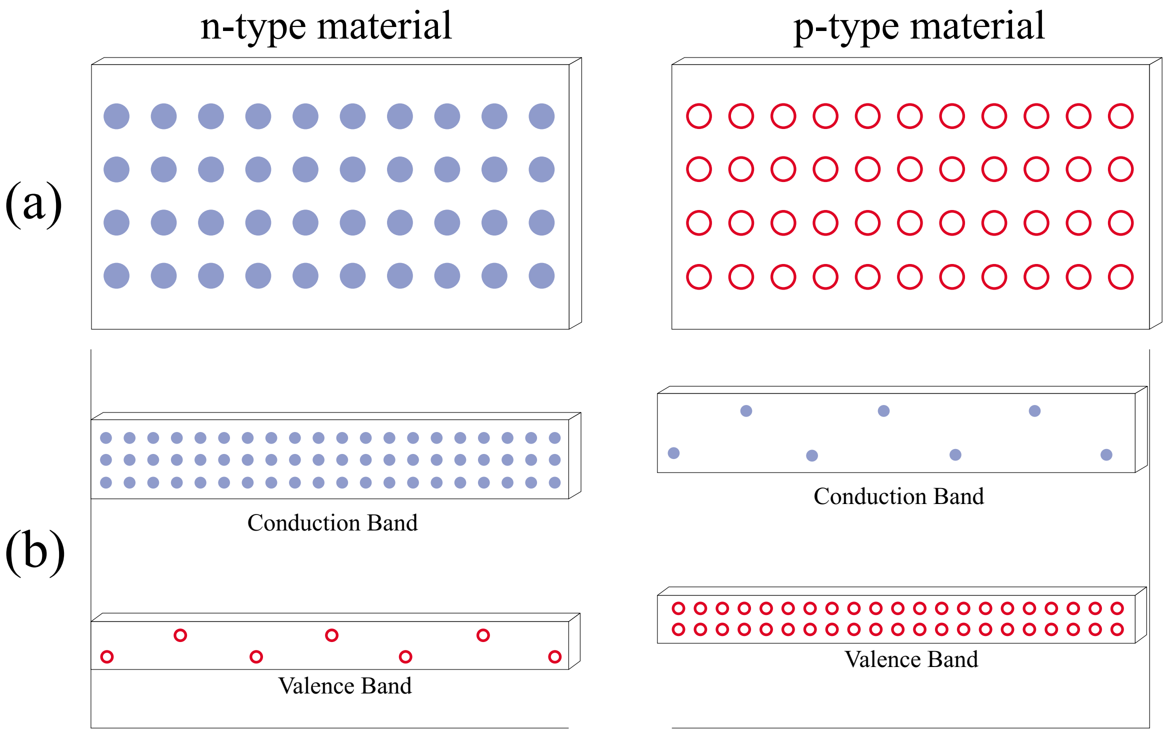


Fig 15 *pn*-junction Initial Energy Levels

The pn Junction

The energy diagrams (Fig 15-b) show the relationship between the energy levels of the two materials. Note that the valence bands of the two materials are at slightly different energy levels as are the conduction bands. This is due to the differences in atomic makeup of the two materials.

Alone, n-type and p-type material are of little use. When they are joined together however, we get an unexpected and useful result. This is done by doping each end of the crystal opposite. One end is doped n-type and the other end is doped p-type. The two types of material are brought together at a defined line in the crystal. Figure 16(a) shows a representation of the doped crystal.

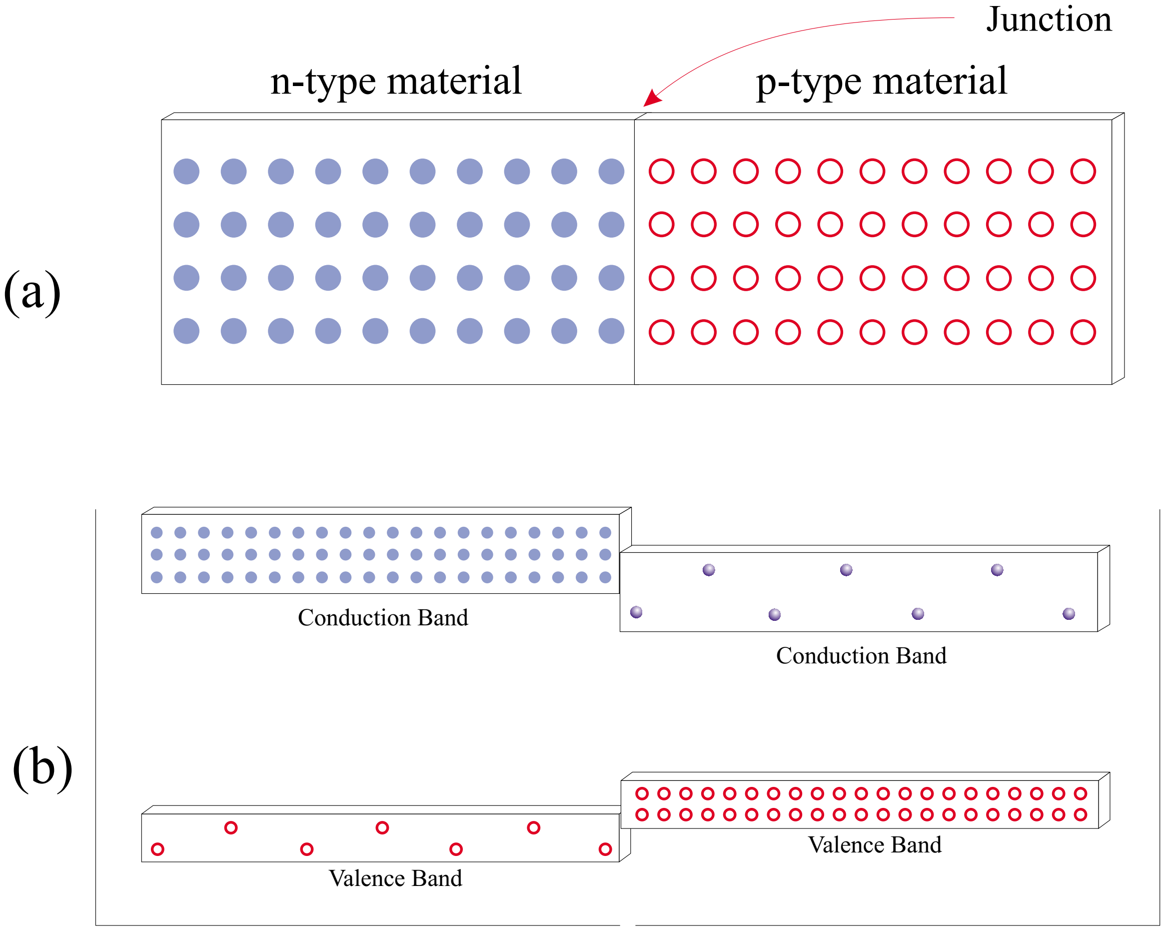


Fig 16 *pn*-junction Initial Energy Levels

Figure 16(b) shows the conduction and valence bands when the materials are joined. Notice that the bands overlap and this allows free electrons from the n-type material to diffuse over to the p- type material. This is when we get an unexpected result.

The Formation of the Depletion Layer

Figure 17 (a) shows the doped crystal and the junction. In the n-type material, there are many free electrons in the conduction band. Some of these electrons will migrate across the junction and enter the p-type material.

When the free electrons migrate across the junction, they will drop from the conduction band and into one of the valence band holes in the p-type material close to the junction. See Fig. 17 (b).

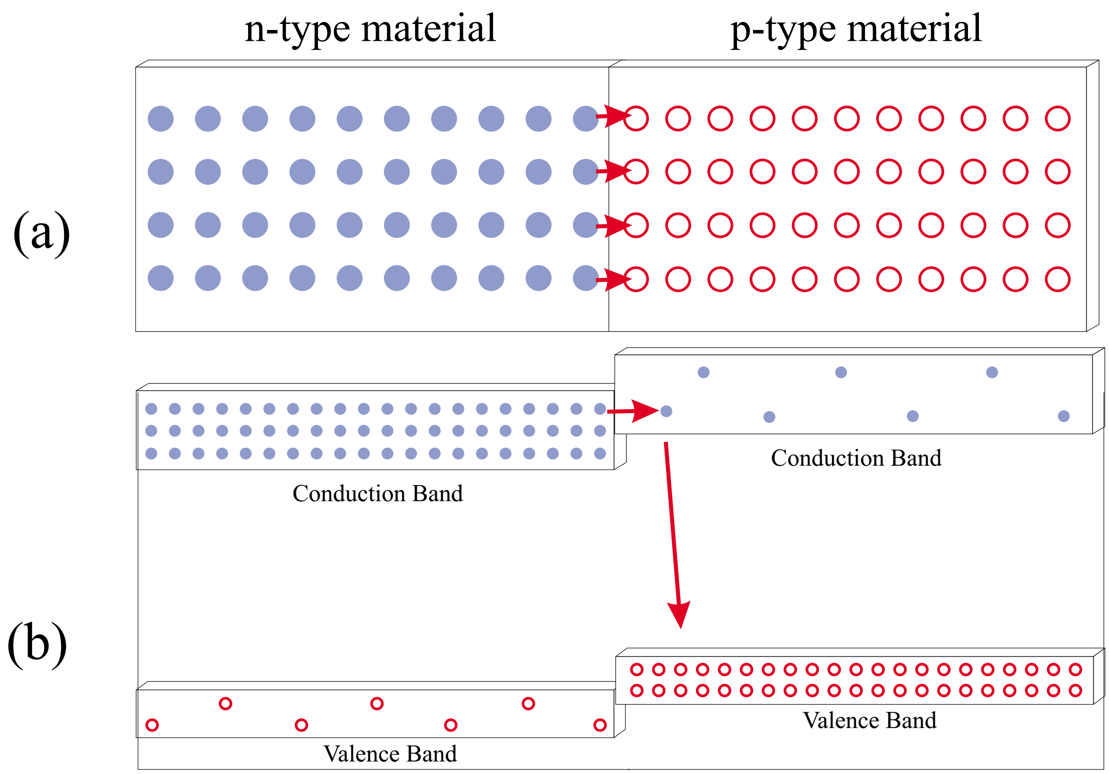


Fig. 17 How the Depletion Layer Forms

Negative Ions

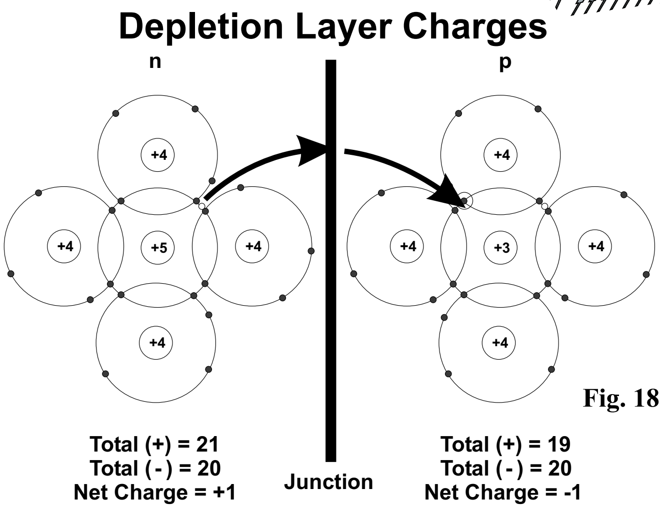


Fig. 18

After the electron drops into the hole, it is locked there and that atom is now a negative ion. As more free electrons cross the junction, they all drop into the valence band in the p-type material. This continues until all of the atoms near the junction in the p-type material have their holes filled. All of these atoms are now negative ions because they all have one extra electron.

At the same time, positive ions are formed n-type side of the junction. For every electron that left the n-side of the junction, a positive ion is formed close to the junction. The number of positive ions will equal the number of negative ions near the junction.

Figure 18 shows this action. For a further description, see section 1.3 in the text.

The Depletion Layer

Remember that negative charges repel. As the number of negative ions increase near the junction, so does the cumulative negative charge. The width of the negative ion area is expanding.

At the same time, the positive ion area is expanding at the same rate. The charge reaches a point where any free electrons that are trying to cross this area are repelled back across the junction. At this point, the growth stops and an equilibrium is reached.

The pn Junction

The Completed Depletion Layer

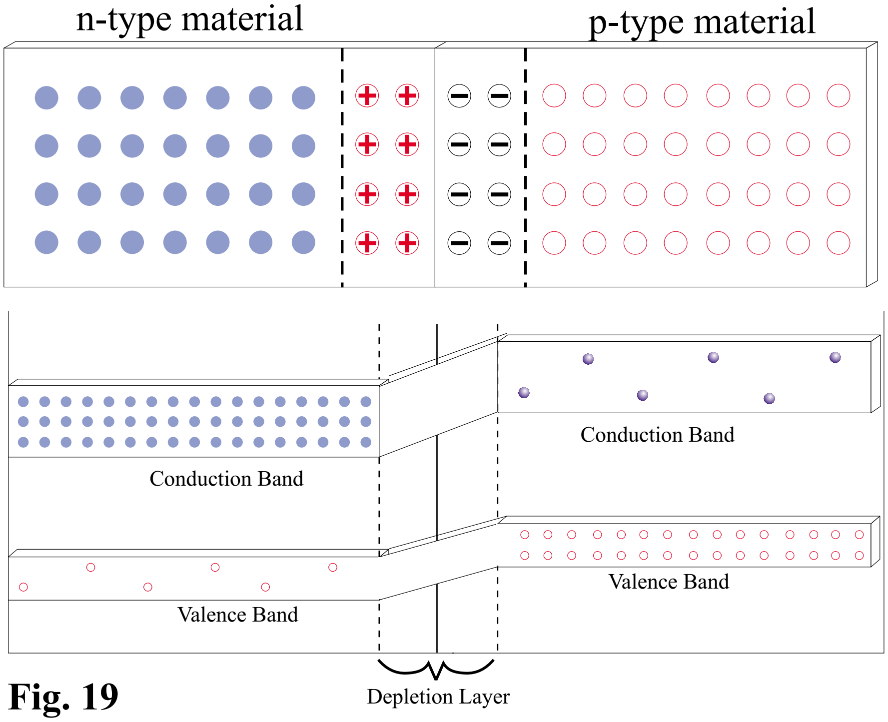


Fig. 19

This area, on both sides of the junction where the ions exist, is called the depletion layer. In this area, only ions exist and they cannot move. Since one side is positive and the other side is negative, a force field is set up between the two (See Figure 19) .This area is depleted of free electrons and holes.

Note that the overall charge of the area is shown to be positive on the n-type side of the junction and negative on the p-type side of the junction.

The Barrier Potential

The n-type side of the junction has a positive potential while the p-type side of the junction has an equal negative potential. You have a natural difference of potential between the two sides of the junction. This potential is referred to as the barrier potential. The barrier potential for **silicon** is approximately **0.7 volts.** For **germanium** it is approximately **0.3 volts.**

The pn Junction

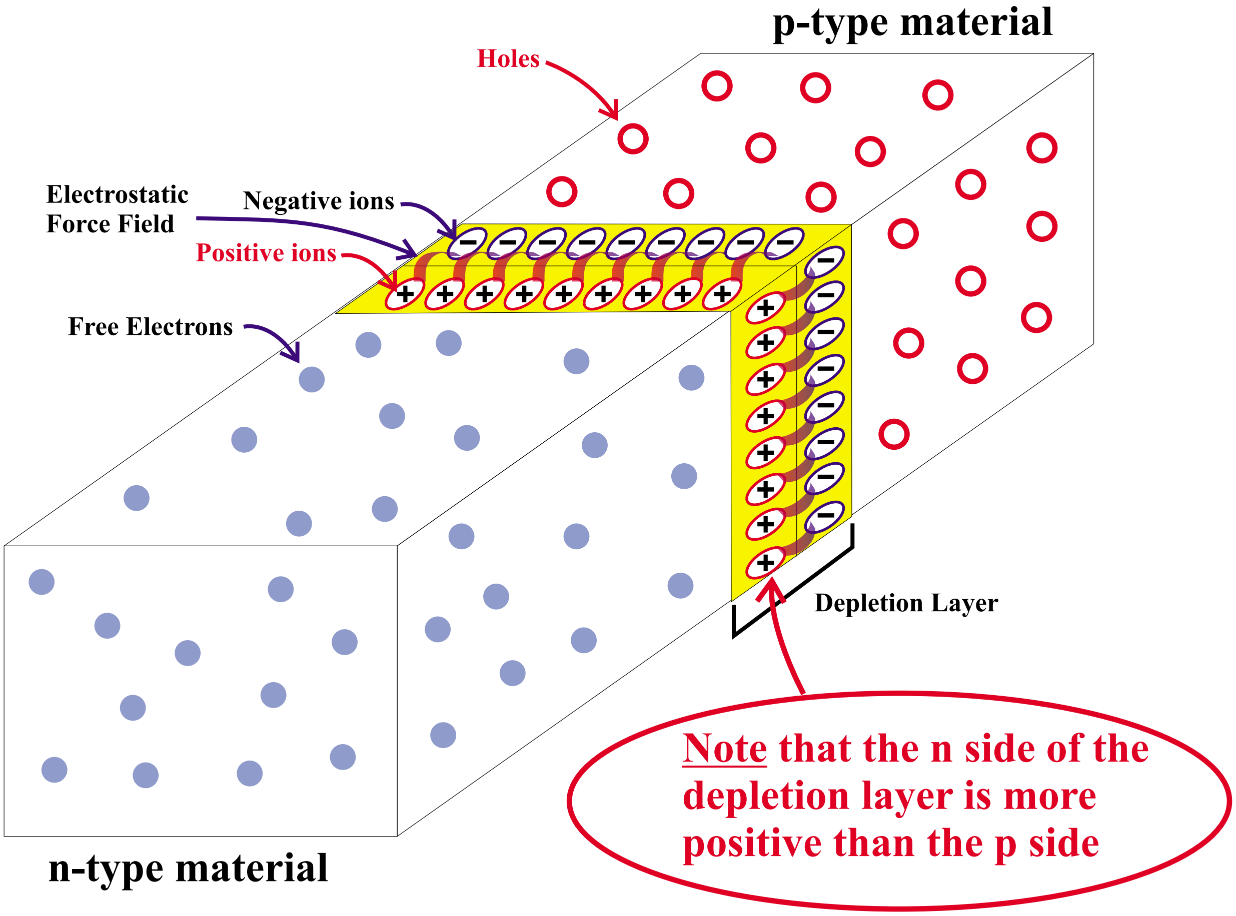


Fig.20 Silicon Crystal depicting the Depletion Layer of the Un-Biased Diode

Controlling the Width of the Depletion Layer

The pn junction becomes useful when we are able to control the width of the depletion layer. By controlling the width, we are able to control the resistance of the pn junction and thus the amount of current that can pass through the device. T he relationship between the width of the depletion layer and junction current is summarized as follows:

Depletion Layer Width	*Junction Resistance*	*Junction Current*
Min.	Min.	Max.
Max.	Max.	Min.

The pn Junction - Forward Bias

Bias

Bias is the potential applied to a pn junction to obtain a desired mode of operation. This potential is used to control the width of the depletion layer. The two types of bias are ***forward bias*** and ***reverse bias***.

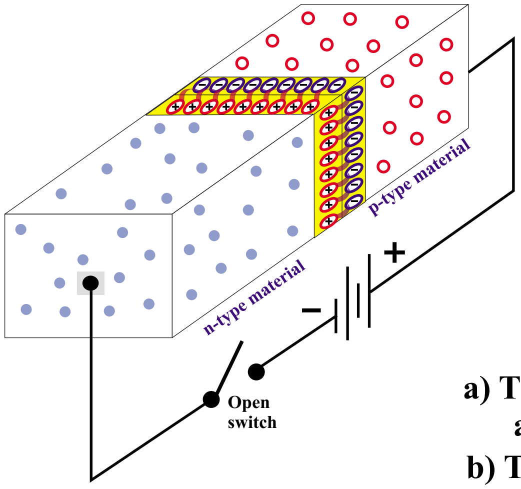
Forward Bias

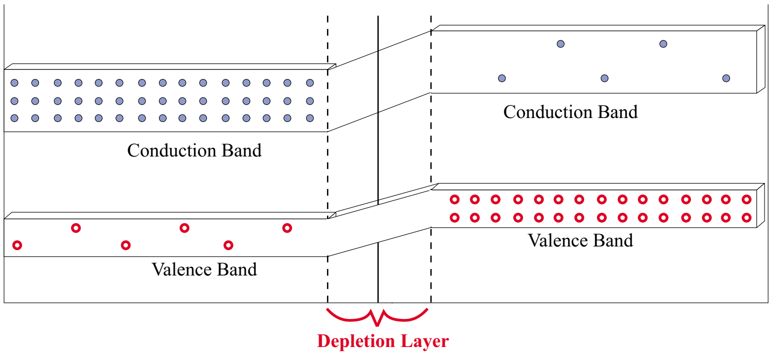
In Figure 21 (a), the diode is unbiased, which means that has no external voltage is being applied to it. The n- type end of the depletion layer is more positive than the p-type end. There are no free electrons or holes in the depletion layer area.

There are small number of free electrons in the p side conduction band caused by heat.

The potential across the depletion layer is approx. ***0.7 Volts for Silicon*** and ***0.3 Volts for Germanium***.

The switch is open and no external voltage is applied to the diode.





a) The depletion layer has formed with the n side positive and the p side negative

b) The barrier potential is approximately 0.7 Volts

Figure 21 (a)

Initial Energy States in the Unbiased Diode

The pn Junction - Forward Bias

Forward Bias (cont)

The moment the switch is closed, a negative potential is applied to the n-type material and a positive potential is applied to the p-type material.

Figure 21 (b) shows the results the moment the switch is closed..

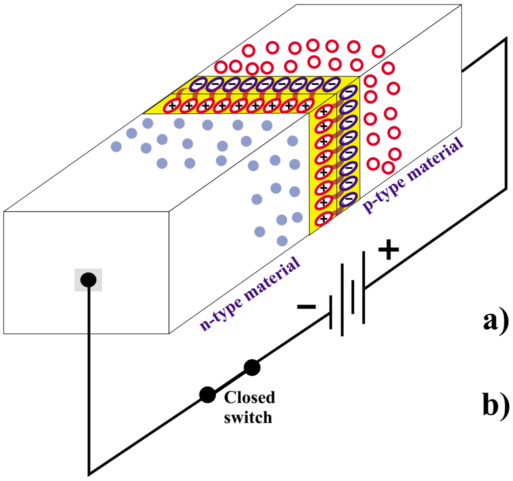
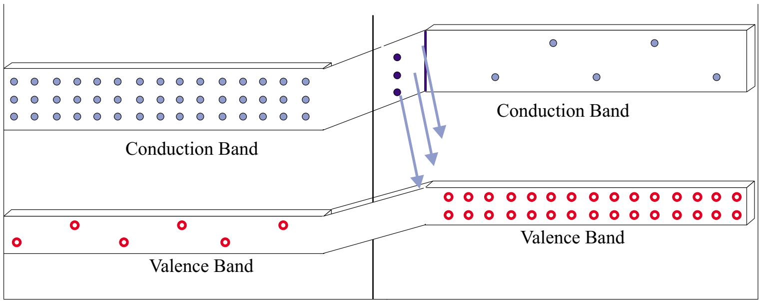


Figure 21 (b)



a) The conduction band electrons in the n-type material are pushed toward the junction by the negative terminal potential

b) The valence band holes in the p-type material are pushed toward the junction by the positive terminal potential

The Moment the Switch is Closed

Figure 21 (c) shows the diode in conduction. The terminal potential must be above 0.7 Volts for conduction to begin.

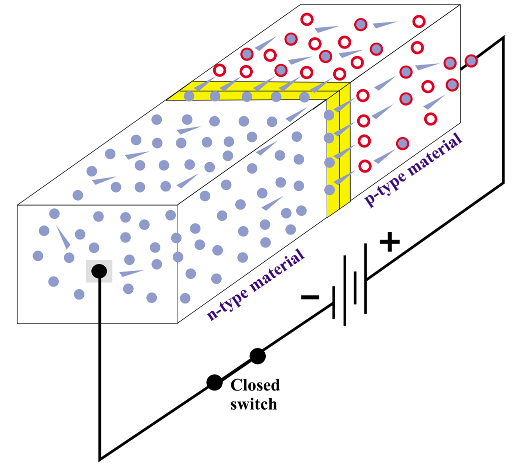
Now electrons have enough energy to overcome the barrier potential and cross over the junction.

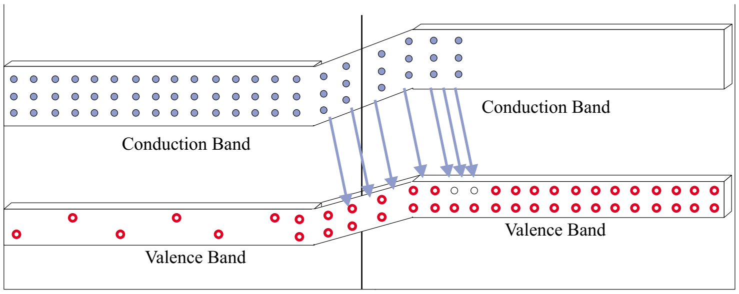
Note that the depletion layer is narrow when conduction occurs .

The majority carriers are the conduction band electrons in the n-type material.

The majority carriers are the valence band holes in the p-type material.

The pn Junction - Forward Bias





a) The terminal potential must be above the barrier potential (0.7V) in order for current to flow across the junction.

b) The electrons will cross the junction and fall into a valence band hole on the p side.

Figure 21 (c) **During Conduction**

Forward Voltage V_F

When a forward biased pn junction begins to conduct, the forward voltage (V_F) across the junction is slightly greater than the barrier potential for the device the values of V_F are ***approximated*** as:

$$V_F = 0.7 \text{ V (Silicon)}$$
$$V_F = 0.3 \text{ V (Germanium)}$$

Bulk Resistance

Once a pn junction is in conduction, it provides a slight opposition to current. This opposition to current is referred to bulk resistance. Bulk resistance is the combined resistance of the n- type and p-type materials. It is written as follows:

$$r_b = r_p + r_n$$

The value of r_b is typically of the range of 25 or less. The exact value of r_b for a given junction depends on the dimensions of the n- type and p- type materials, the amount of doping used to produced materials, and the operating temperature. Since r_b is generally small, it is often ignored in circuit calculations.

Forward Biasing a pn Junction

There are two ways to forward bias a pn junction.

1) By applying a potential to the n-type material that is more negative than the p-type material potential.

2) By applying a potential to the p-type material that is more positive than the n-type material potential.

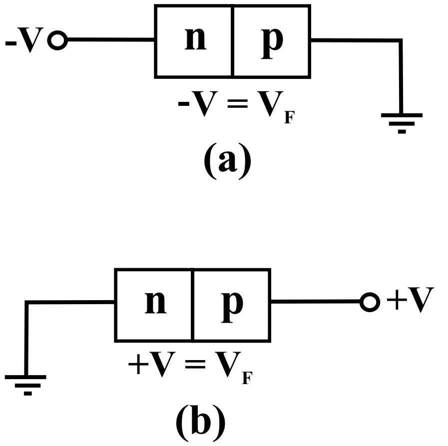


Fig 22

Figure 22 illustrates these two biasing methods. The grounded end of the diodes are at zero volts.

In Figure (a), the p-type material is at zero volts. In order for the junction to conduct the n-type material must be at a potential of greater than **- 0.7 volts**.

In Figure (b), the n-type material is at zero volts. In order for the junction to conduct the p-type material must be at a potential of greater than **+ 0.7 volts**.

In either case, as far as the junction is concerned, it will conduct if two criteria are met.

- It must see a potential across itself of greater than 0.7 volts
- The polarity of this potential must be: - p-side more positive than the n-side.

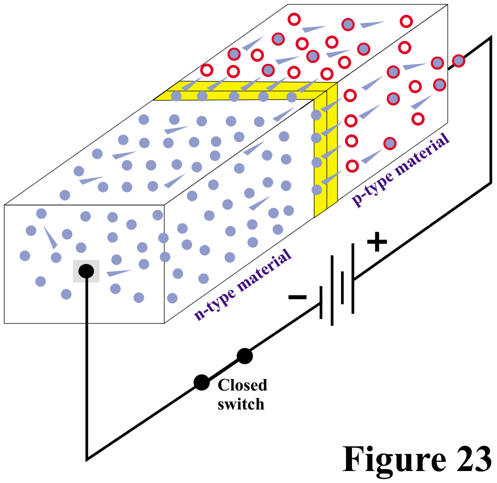
A further explanation is in the text in Section 1.4

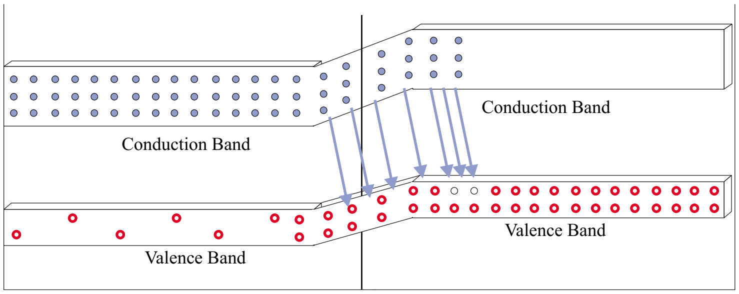
The pn Junction - Reverse Bias

Reverse Bias

A pn junction is reversed biased when the applied potential causes the n-type material to be more positive the p-type material. The depletion layer becomes wider and almost no current will flow. Figure 23 shows the effects of reverse bias.

Figure 23 (a) shows the forward biased diode as before. The depletion layer is narrow and the diode is allowing current pass with little opposition.

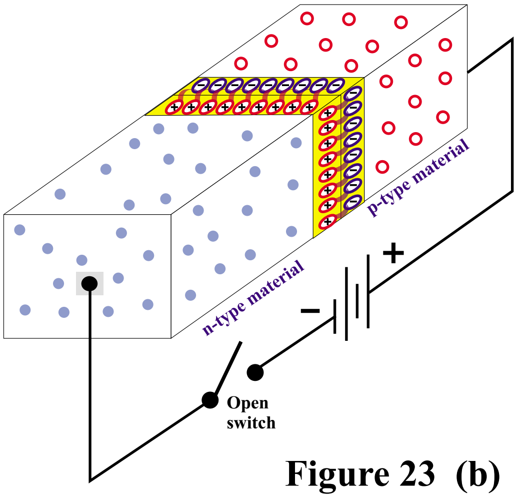


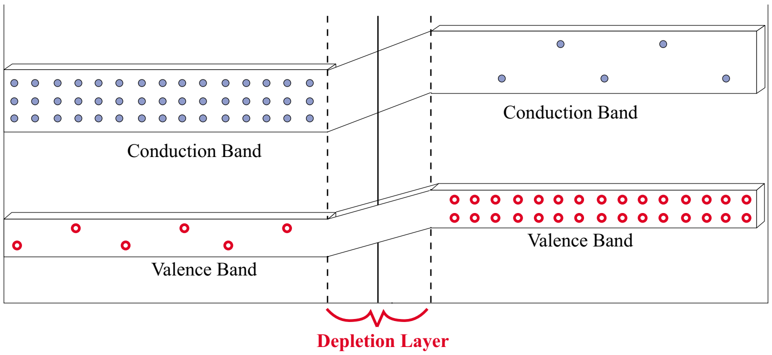


The depletion layer is narrow & there is little opposition to current flow.

Figure 23 (a) **The Forward Biased Diode**

Figure 23 (b) shows the diode with the switch open. The diode is no longer forward biased and the depletion layer re-forms as electrons diffuse across the junction.





The depletion layer re-forms when the switch is opened and the diode returns to its un-biased state

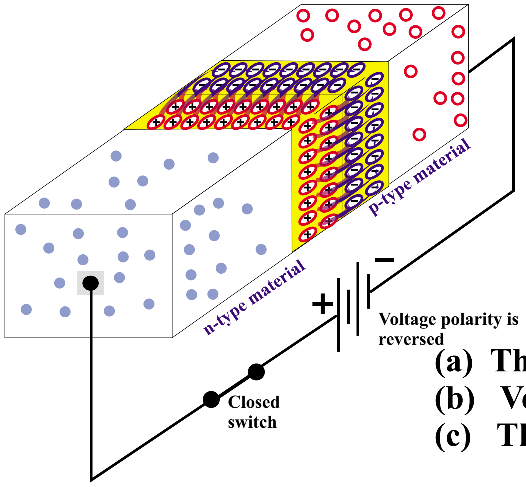
Figure 23 (b) **The Depletion Layer returns - The unbiased Diode**

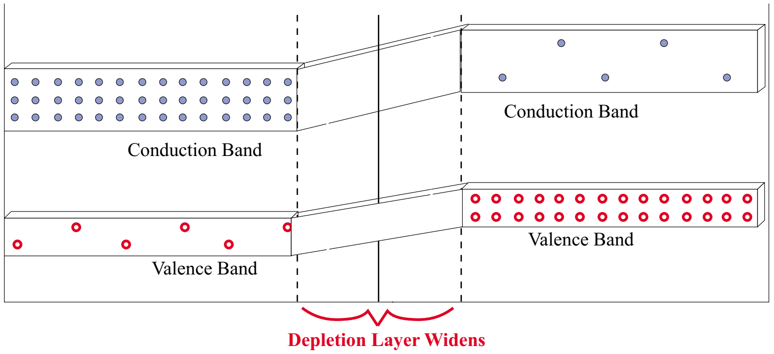
The pn Junction - Reverse Bias

Figure 23 (c) shows the diode in reverse bias. Notice that the power supply is now reversed. When the switch is closed the electrons in the n-type material head towards positive terminal. At the same time, the holes in the p-type material move towards the negative terminal.

The electron movement away from the n-side of the junction further depletes the material of free carriers. The depletion layer has effectively been widened.

The same principle takes place on the p-side of the material. Since there are fewer holes near the junction, the depletion layer has grown. The overall effect of the widening of the depletion layer is that the resistance of the junction has been dramatically increased, and conduction drops to near zero.





(a) The depletion layer widens as the reverse potential is increased
(b) Very little current flows across the junction
(c) The free electrons & holes move away from the junction

Figure 23 (c)

The Reverse Biased Diode

Diffusion Current

During the time that the depletion layer is forming and growing, there is still majority carrier current in both materials. This diffusion current last only as long as it takes the depletion layer to reach its maximum width.

The pn Junction - Reverse Bias

Diffusion current is undesirable in high frequency circuits, so special diodes have been developed for these types of circuits.

Reverse Biasing a pn Junction

There are two ways to reverse bias a pn junction.

1) By applying a potential to the n-type material that is more positive than the p-type material potential.

2) By applying a potential to the p-type material that is more negative than the n-type material potential.

Summary

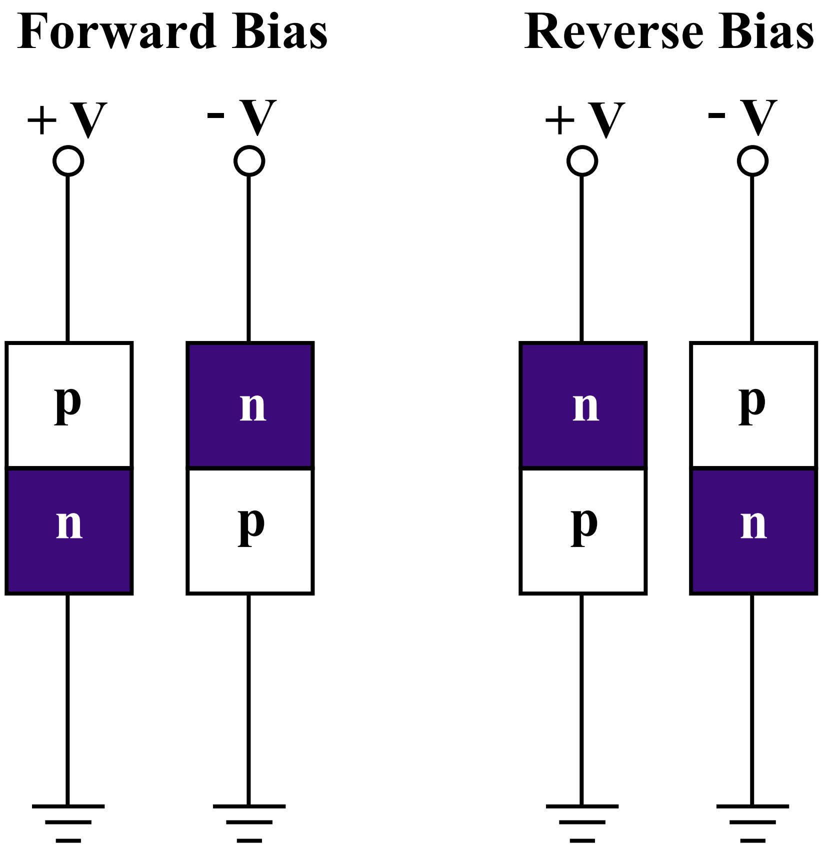
Bias is a potential applied to a pn junction that determines the operating characteristics of the device. Bias polarities and effects are summarized as follows:

Bias Type	Junction Polarities	Junction Resistance
Forward	n-type material is more (-) than p-type material	Extremely low
Reverse	p-type material is more (-) than n-type material	Extremely high

Forward Bias Voltage Drop V_F
Silicon $\cong$ 0.7 V
Germanium $\cong$ 0.3 V

The pn Junction - Summary

Bias Polarities



Depletion Layer Width:	**Minimum**	**Maximum**
Device Resistance:	**Minimum**	**Maximum**
Device Current:	**Maximum**	**Minimum**

Please read Chapter 1 and the Chapter Summary in the text