CAREER COLLEGE BHOPAL

Solid State Physics and Electronic Device

Solid State Physics-1

Lecture-5

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Contents:

- Band Theory of Solids
- Periodic Potential
- Bloch Theorem
- Kronig Penny Model

Band Theory of Solids

A useful way to visualize the difference between conductors, insulators and semiconductors is to plot the available energies for electrons in the materials. Instead of having discrete energies as in the case of free atoms, the available energy states form bands. Crucial to the conduction process is whether or not there are electrons in the conduction band.

In insulators the electrons in the valence band are separated by a large gap from the conduction band, in conductors like metals the valence band **overlaps** the conduction band, and in semiconductors there is a small enough gap between the valence and conduction bands that thermal or other excitations can bridge the gap. With such a small gap, the presence of a small percentage of a doping material can increase **conductivity** dramatically.

An important parameter in the band theory is the Fermi level, the top of the available electron energy levels at low temperatures. The position of the Fermi level with the relation to the conduction band is a crucial factor in determining electrical properties.

The energy band structure of a solid determines whether it is a conductor, an insulator or a semiconductor. A solid contains an enormous number of atoms packed closely together. Each atom, when isolated, has a discrete set of electron energy levels 1s,2s,2p,..... If we imagine all the N atoms of the solid to be isolated from one another, they would have completely coinciding schemes of their energy levels.

Let us study what happens to the energy levels of an isolated atom, as they are brought closer and closer together to form a solid. If the atoms are brought in close proximity, the valence electrons of adjacent atoms interact. Hence the valence electrons constitute a single system of electrons common to the entire crystal with overlapping of their outermost electronic orbits. Therefore, the N electrons will now have to occupy different energy levels.

This is brought about by the electric forces exerted in each electron by all the N nuclei. As a result of these forces, each atomic energy level is split up into a large number of closely spaced energy levels. A set of such closely spaced energy levels is called an energy band. For example, the 11 electrons in a neutral sodium atom, each occupy a specific energy level.

The energy levels of sodium become bands when the atoms are close together. In figure r0 is the distance between the atoms in solid sodium. When the atoms are in solid, they interact with each other and the electrons have slightly different energies. In the energy band, the allowed energies are almost continuous. These energy bands are in general, separated by regions, which have no allowed energy levels.

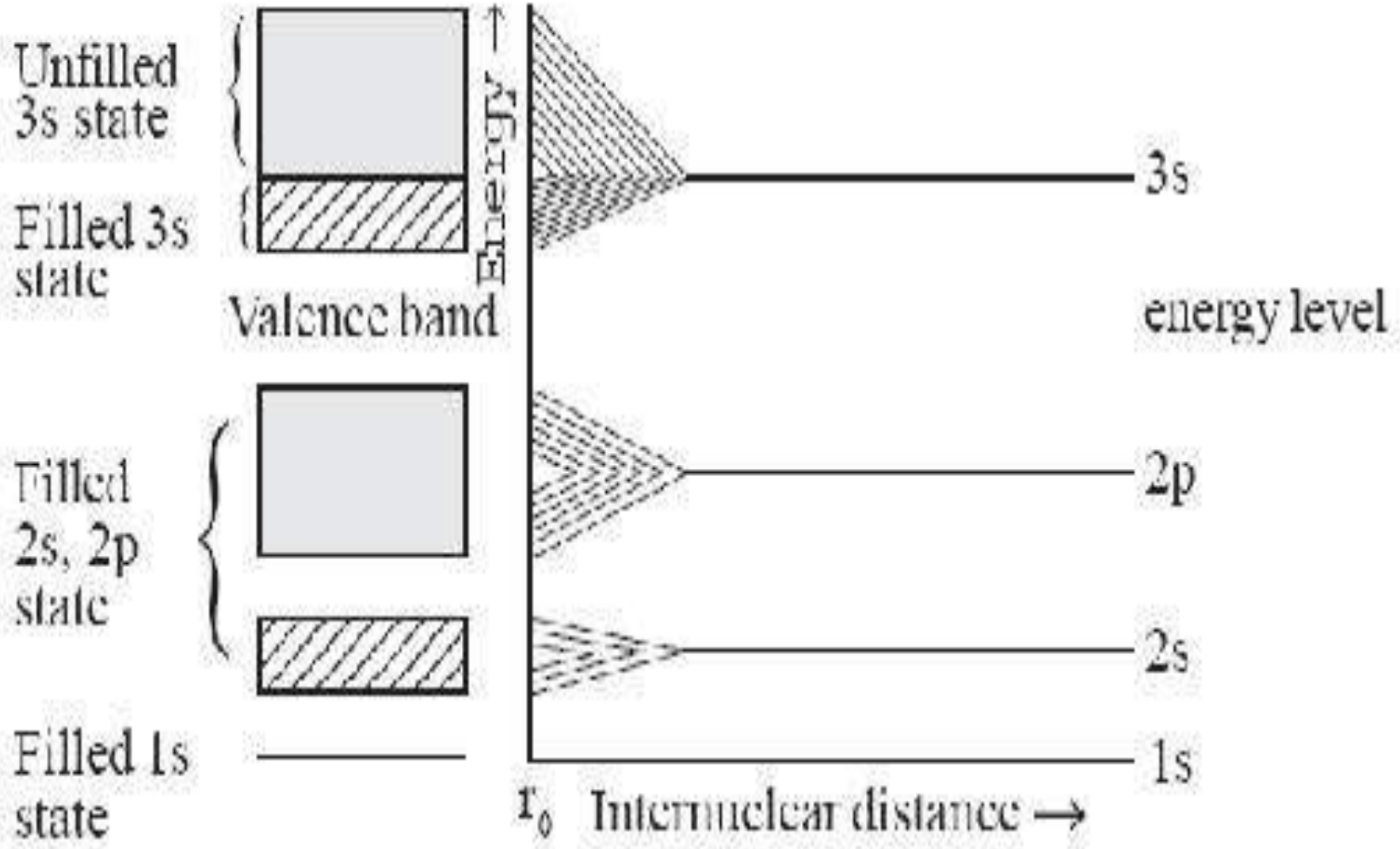
These regions are known as "forbidden bands" or 'energy gaps'. The amount of splitting is not the same for different levels. The levels filled by the valence electrons in an atom are disturbed to a greater extant, while those filled by inner electrons are disturbed only slightly.

If there are N atoms in a solid, there will be N allowed quantum states in each band.

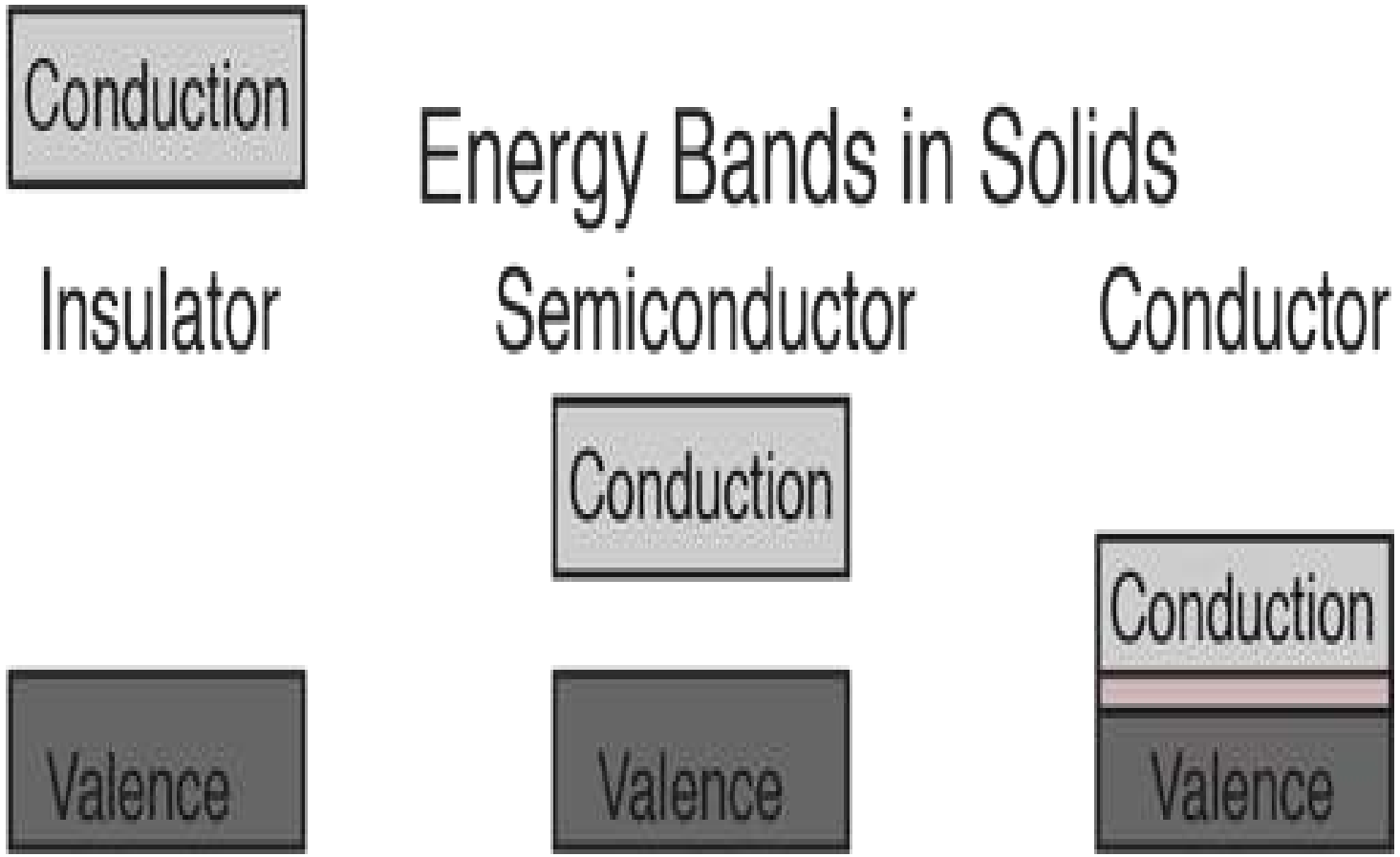
Each quantum state can be occupied by a maximum of two electrons with opposite spins. Thus each energy band can be occupied by **2N electrons**. The band formed from the atomic energy levels containing **valance electrons** is called valance band. These electrons have the highest energy. Above the valance band, there is the band of next higher permitted energies called the 'conduction band'.

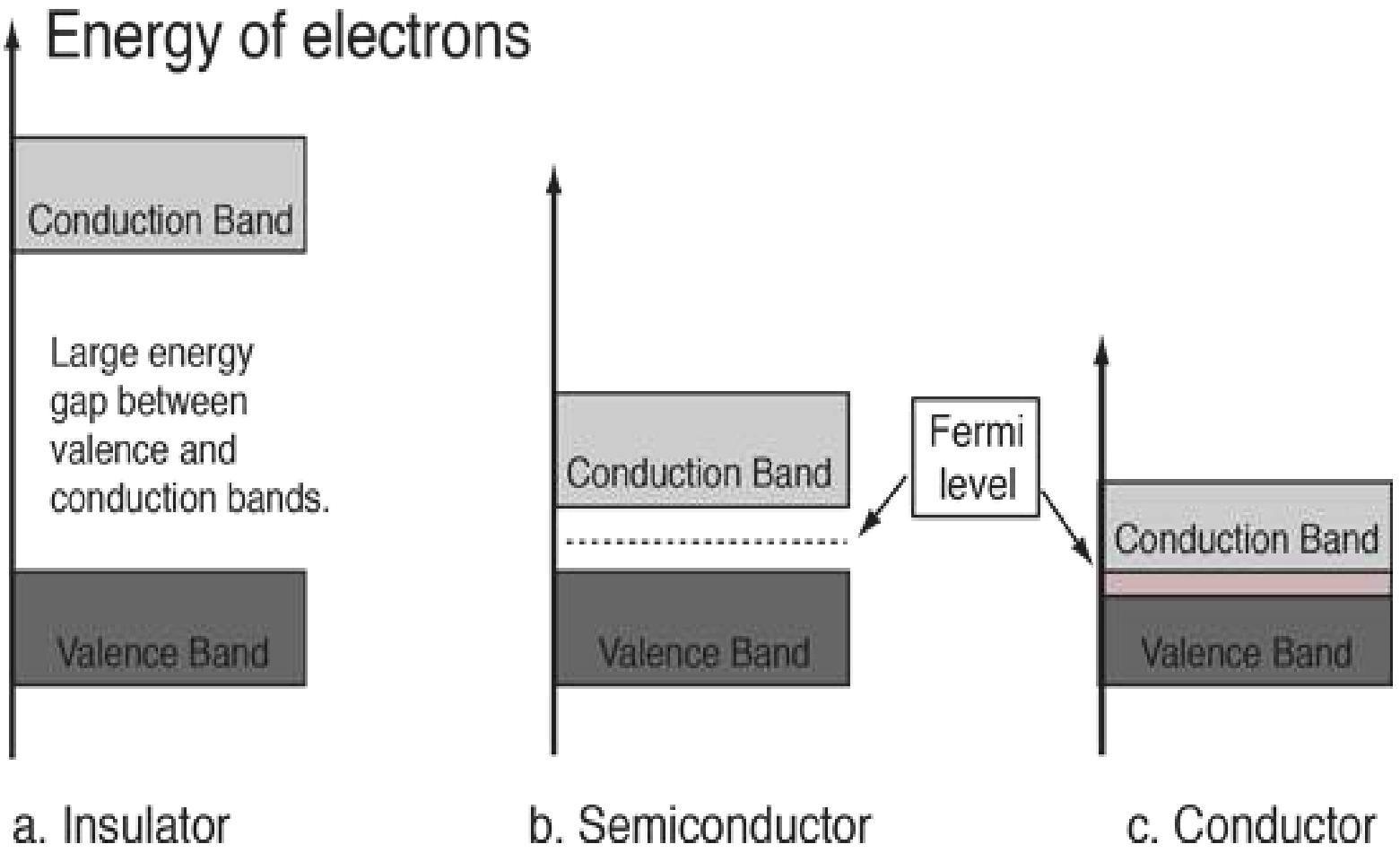
The conduction band corresponds to the first excited states; electrons can move freely in this band and are called 'conduction electrons'.

The interval between conduction band and valence band in which electrons cannot occupy is called 'Forbidden gap'.


Unfilled
3s state
Filled 3s
state
Valence band
Energy →
3s
energy level
Filled
2s, 2p
state
2p
2s
Filled 1s
state
1s
r_0 Internuclear distance →

Energy Bands in Solids



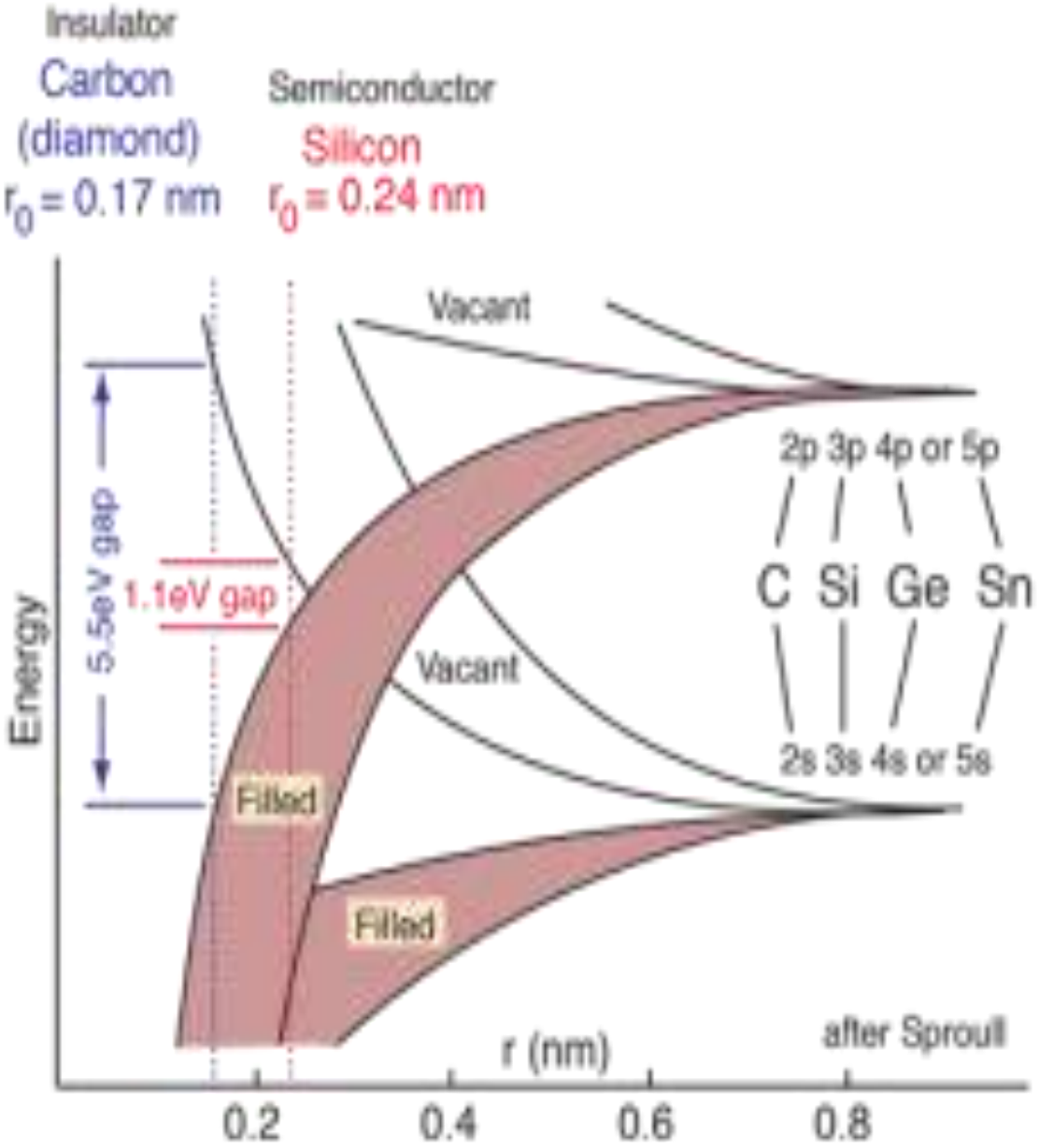

Energy of electrons
Conduction Band
Large energy gap between valence and conduction bands.
Valence Band
Conduction Band
Fermi level
Valence Band
Conduction Band
Valence Band
a. Insulator
b. Semiconductor
c. Conductor

Energy Bands : Insulators and Semiconductors:

The energy bands for the outermost electrons are qualitatively similar for carbon, silicon, germanium and tin. Though they will differ in detail, the generic band diagram below can show why these materials have different electrical properties.

Periodic table environment of semiconductors

B	C $2p^2$	N
Al	Si $3p^2$	P
Ga	Ge $4p^2$	As
In	Sn $5p^2$	Sb
Tl	Pb $6p^2$	Bi

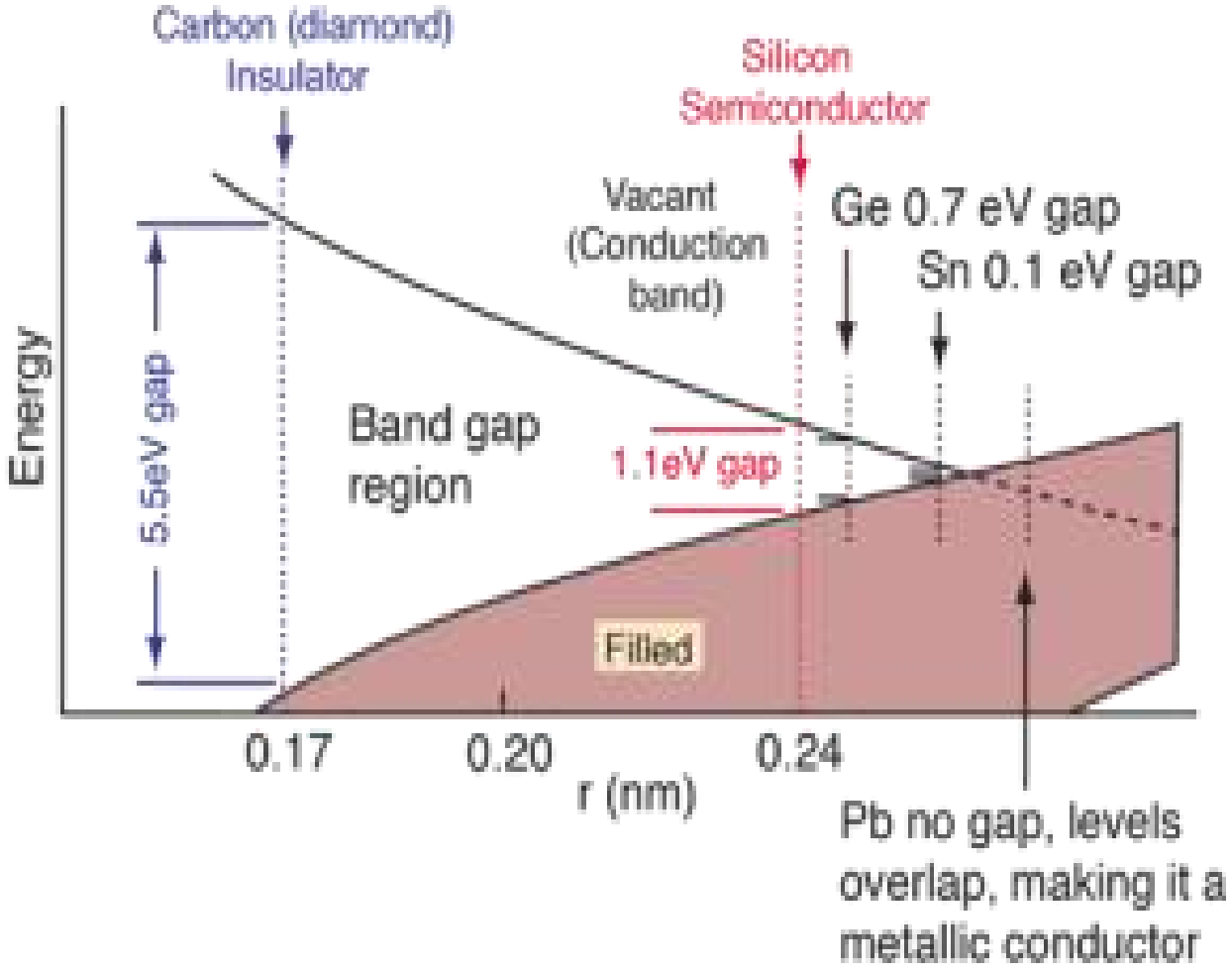


Inter-atomic spacing and semiconductors:

The energy bands for the outermost electrons are qualitatively similar for carbon, silicon, germanium and tin. The diagram shows that there is a strong correlation between the inter-atomic spacing and the electrical properties of the solid.

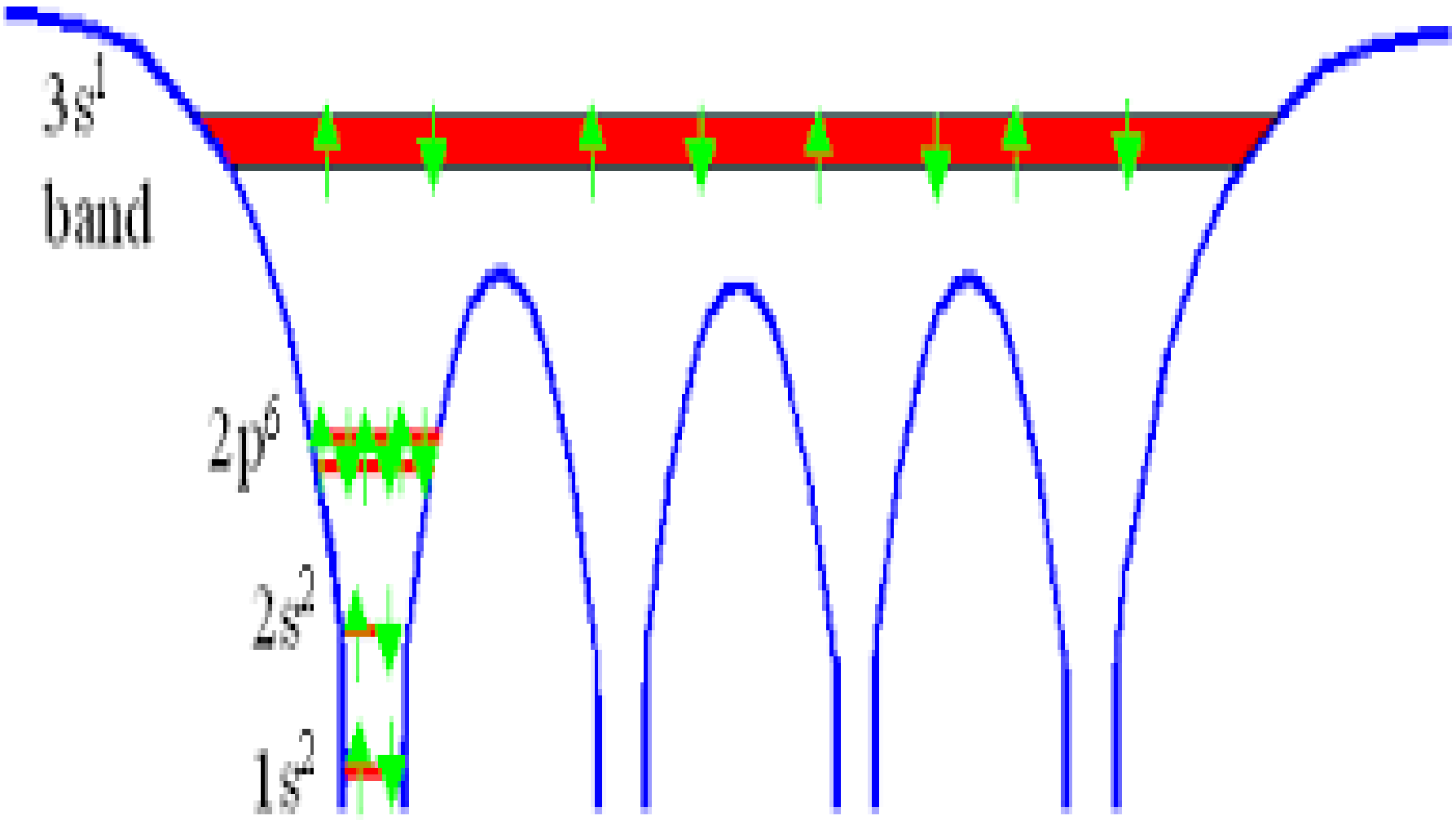
Periodic table environment of semiconductors

B	C $2p^2$	N
Al	Si $3p^2$	P
Ga	Ge $4p^2$	As
In	Sn $5p^2$	Sb
Tl	Pb $6p^2$	Bi



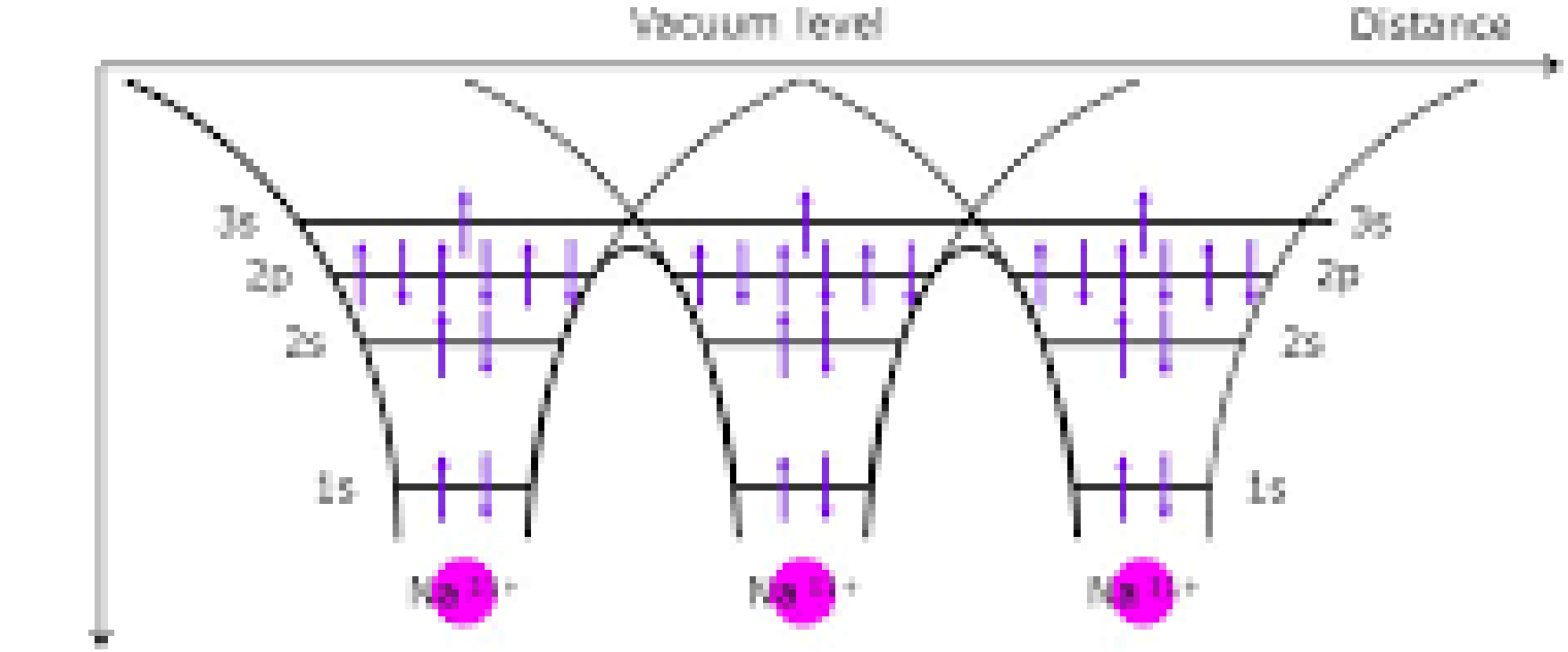
Periodic Potential:

In quantum mechanics, the particle in a one-dimensional lattice is a problem that occurs in the model of a **periodic** crystal lattice. The **potential** is caused by ions in the **periodic** structure of the crystal creating an electromagnetic field so electrons are subject to a regular **potential** inside the lattice.


$3s^1$
band
$2p^6$
$2s^2$
$1s^2$

Periodic Potential in a Crystal

Potential energy in a crystal (e.g., *N* Na atoms) :



- Potential energy changes the shape inside a crystal.
- 3s state forms *N* energy levels → Conduction band

Bloch's Theorem

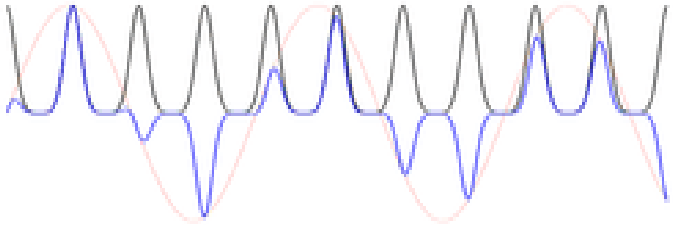
$$\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

- Independent electrons which obey the one electron Schrödinger equation for a periodic potential are called *Bloch electrons* and obey Bloch's theorem

$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

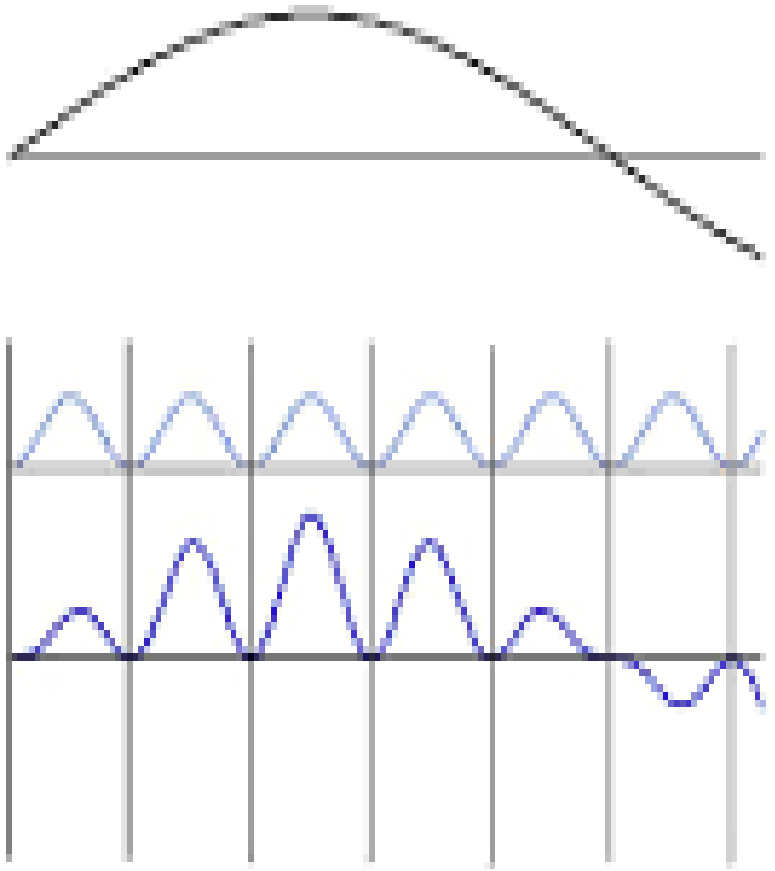
- Bloch's theorem can be written in two equivalent forms

$$\Psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \Psi_{n\mathbf{k}}(\mathbf{r})$$



Bloch theorem visualization

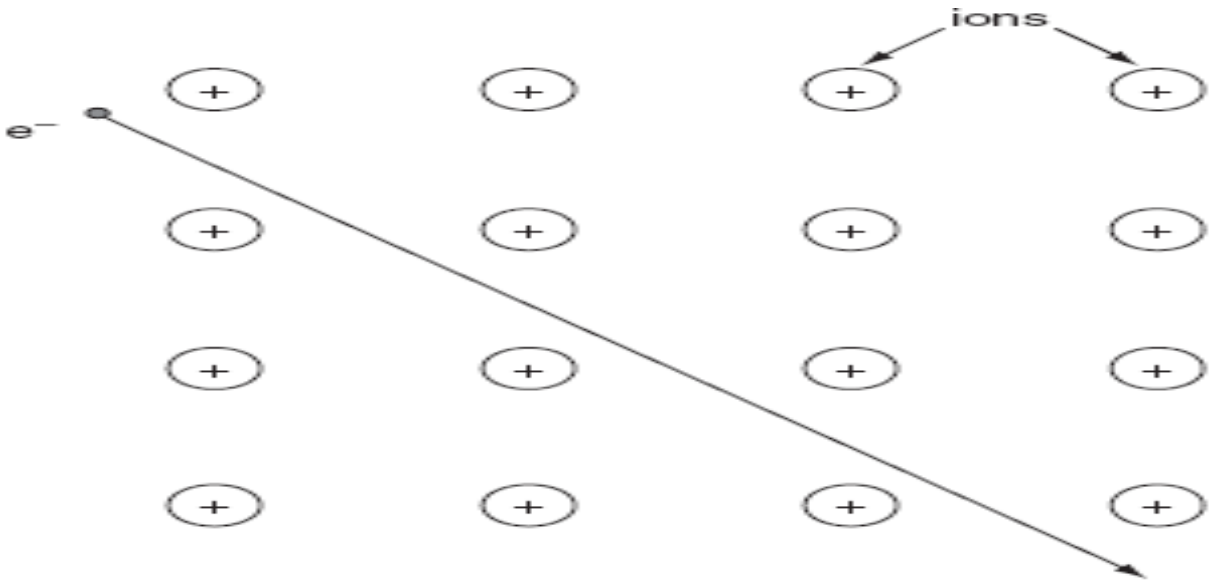
Visualization of the real part of the wavefunction



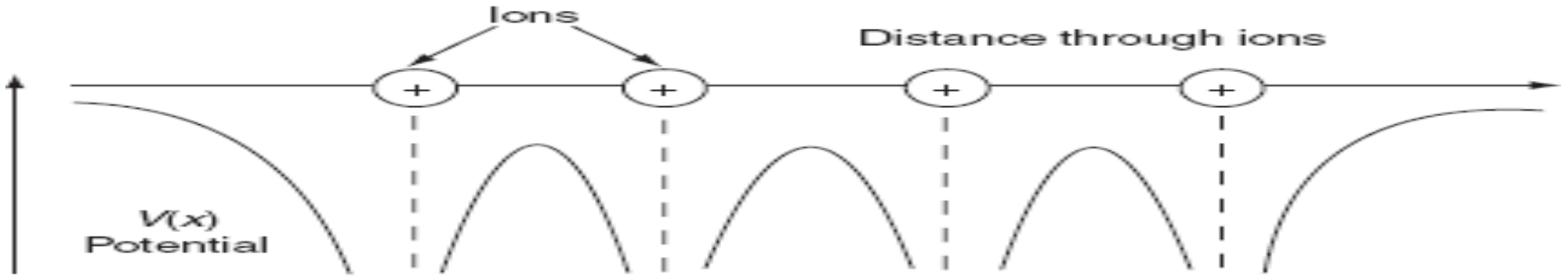
Kronig Penny Model

- According to quantum free electron theory of metals, a conduction electron in a metal
- experiences constant (or zero) potential and free to move inside the crystal but will
- not come out of the metal because an infinite potential exists at the surface.
- This theory successfully explains electrical conductivity, specific heat, thermionic emission and para-magnetism.
- This theory is fails to explain many other physical properties, for example:

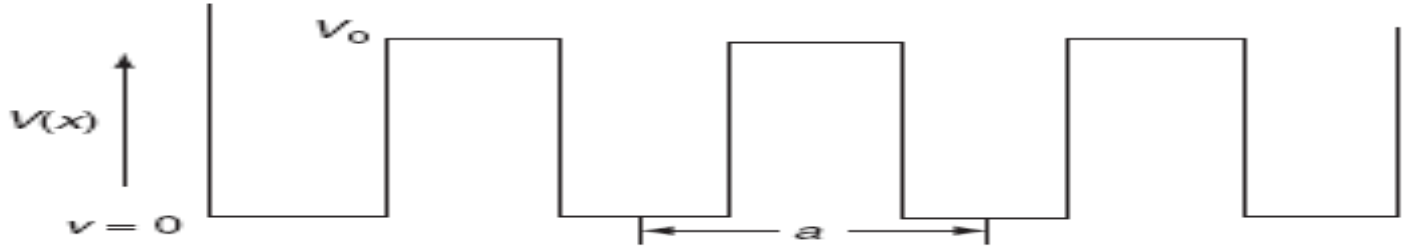
- (i) it fails to explain the difference between conductors, insulators and semiconductors, (ii) positive Hall coefficient of metals and (iii) lower conductivity of divalent metals than mono-valent metals.
- To overcome the above problems, the periodic potentials due to the positive ions in a metal have been considered.
- shown in Fig. (a), if an electron moves through these ions, it experiences varying potentials. The potential of an electron at the positive ion site is zero and is maximum in between two ions. The potential experienced by an electron, when it passes along a line through the positive ions is as shown in Fig. (b).



(a)



(b)



(c)

THANK YOU