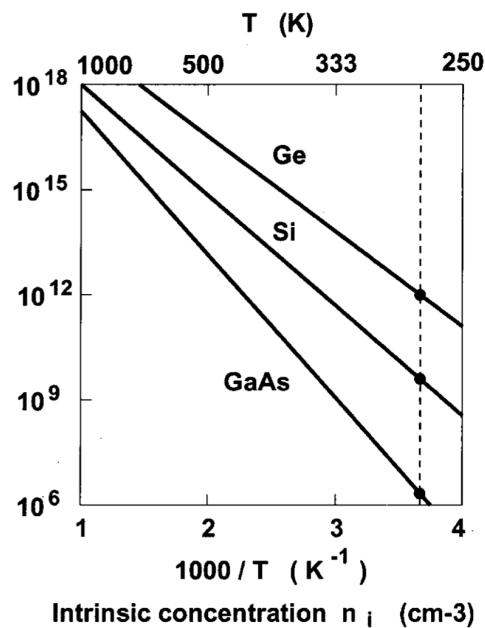


## Lecture-5

Continuing from Lecture-4

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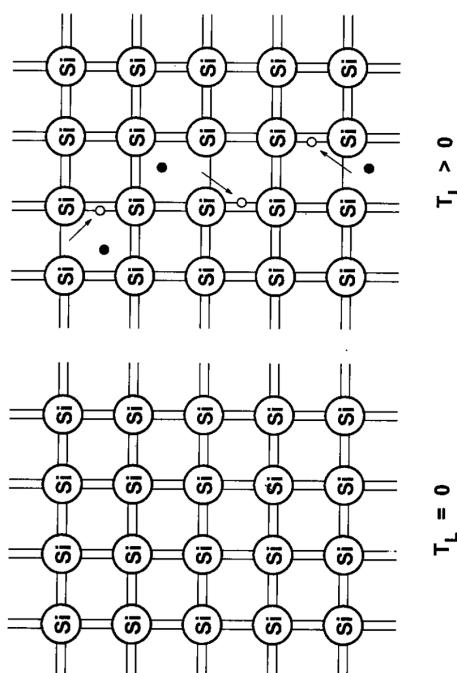
- The above figure represents Intrinsic Concentration at equilibrium in a Semiconductor as a function of Temperature.
- This is a special graph where concentration is indicated in logarithmic scale and the horizontal axis instead of reporting Temperature has inverse of Temperature. In this way we have a graph which is essentially a straight line. This type of Diagram has got a Name.

i.e  $\log(n_i)$  Inverse of a variable

function  
is called Arrhenius plot  
↓  
Name of a scientist with Nobel prize  
in CHEMISTRY in late 1800's



T. 22.14: Rappresentazione bidimensionale del silicio intrinseco.

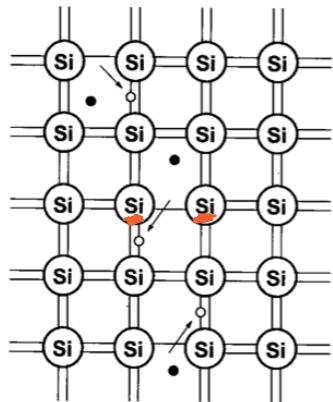


→ Here,  
pictorial representation  
of a silicon crystal  
instead of Energy is  
used.

→ we know that Si belongs  
to column IV of periodic  
Table.  
for this reason Si has  
14 electrons in external  
shell. It can bond  
4 bonds with other  
Si atoms.

Here we will analyze 2D array of silicon crystal.

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$$T_L > 0$$

For Temperature  
 $> 0^\circ\text{K}$

\* The Si-Si pair of sticks  
two electrons that form  
covalent bonding b/w two Si atoms.

Each stick corresponds to  
ONE electron, we know that  
electrons are indistinguishable.  
from each other.

$\therefore$  we can say pair of sticks  
i.e. electrons belongs to  
both atoms.



- $\rightarrow$  Free Electron ( Each Free electron is free to go everywhere in the crystal, Lattice motion is random, if we take Average Energy of all Free electrons in equilibrium turns out to be zero)
- $\rightarrow$  Holes

$\rightarrow$  In This picture we can see absence of a stick b/w two silicon atoms because of electron scattering free.  $\therefore$  There is a disturbance of electric potential in the vicinity of two Si atoms, which is different from original case.

$\rightarrow$   $\therefore$  There is a greater chance of electron in the vicinity of missing stick to perform Tunneling i.e. to go and replace the missing stick.

which is indicated in the figure as

Hole moving from missing stick to wire  
New electron comes from.

Tunnel Effect is a Quantum Effect -

We choose it as motion of hole instead of electron for our convenience

Note:- As long as we are in equilibrium we have  
No current bcs average Velocity of e<sup>-</sup>s  
at holes is zero

### Electron Average Velocity

$$\mathbf{v}_{nj}(\mathbf{r}, t) = \frac{\int_{(j)} \mathbf{u}(\mathbf{k}) Q \Phi(\mathbf{r}, \mathbf{k}, t) d^3k}{\int_{(j)} Q \Phi(\mathbf{r}, \mathbf{k}, t) d^3k} = \frac{\int_{(j)} \mathbf{u} Q \Phi d^3k}{n_j}$$

↓ Distribution Function

Properties

Individual velocity of each electron  $\mathbf{u}(\mathbf{k})$   
Density of states  $Q$  per unit volume  $d^3k$   
Distribution function in the space of  $(\mathbf{r}, \mathbf{k})$  in the space of  $\mathbf{k}$

It is a vector

- A band with no electrons ( $\Phi \equiv 0$ ) has  $n_j \mathbf{v}_{nj} = 0$ .

- A band in which every state is filled with an electron has  $\mathbf{v}_{nj} = 0$  because  $\Phi \equiv 1$ ,  $\mathbf{u}(\mathbf{k})$  is odd, and the first Brillouin zone is centered on the origin.

- In equilibrium it is  $\mathbf{v}_{nj} = 0$  because  $\Phi = P(\mathbf{r}, E)$ ,  $E(\mathbf{k})$  is even,  $\mathbf{u}(\mathbf{k})$  is odd, and the first Brillouin zone is centered on the origin.

- The charge density due to the electrons of the  $j$ th band is  $\rho_{nj} = -qn_j$ ,  $q = 1.602 \times 10^{-19}$  C. The current density is  $\mathbf{J}_{nj} = \rho_{nj} \mathbf{v}_{nj} = -qn_j \mathbf{v}_{nj}$ .

$u(k)$ : Velocity of electron that belongs to state ' $k$ ' of the Brillouin zone and this  $\textcircled{u}$  is related to the branch of energy  $E(k)$

→ when we are integrating over ' $k$ ' we must remember considering one Branch at a time.

In the equation we have a Branch of index  $\textcircled{j}$

$$v_{nj}(r, t) \doteq \frac{\int_{(j)} u(k) Q\Phi(r, k, t) d^3k}{\int_{(j)} Q\Phi(r, k, t) d^3k} = \frac{\int_{(j)} u Q\Phi d^3k}{n_j}$$



This is the Average velocity of Electrons of  
Band no.  $\textcircled{j}$

' $n$ ' reminds us that we are talking about electrons.

It's electrons because we are using distribution function of electrons

→ Index  $j$  reminds us that we are using only one band of index  $j$ .

Obviously distribution function also depends on  $\mathbf{r}$  &  $t$  in general. After integrating over ' $k$ ' we expect that Avg. Velocity will depend on  $\mathbf{r}$  &  $t$

### Properties

- A band with no electrons ( $\Phi \equiv 0$ ) has  $n_j \mathbf{v}_{nj} = 0$ .
- A band in which every state is filled with an electron has  $\mathbf{v}_{nj} = 0$  because  $\Phi \equiv 1$ ,  $\mathbf{u}(\mathbf{k})$  is odd, and the first Brillouin zone is centered on the origin.
- In equilibrium it is  $\mathbf{v}_{nj} = 0$  because  $\Phi = P(\mathbf{r}, E)$ ,  $E(\mathbf{k})$  is even,  $\mathbf{u}(\mathbf{k})$  is odd, and the first Brillouin zone is centered on the origin.
- The charge density due to the electrons of the  $j$ th band is  $\rho_{nj} = -qn_j$ ,  $q = 1.602 \times 10^{-19}$  C. The current density is  $\mathbf{J}_{nj} = \rho_{nj} \mathbf{v}_{nj} = -qn_j \mathbf{v}_{nj}$ .

From The Equation

$$\nabla_{nj} (\mathbf{r}, t) \cdot \mathbf{n}_j = \int_{(j)} u \Phi d^3 k$$

↳  $\rho_0 - 1$

↓  
product of Velocity and Concentration  
↔ ↔ ↔

→ The above properties are based on the equation we just manipulated.

(i) if

$$\phi = 0$$

i.e probability  
is zero for a  
Band with No electrons

we can say intuitively this is Flux

$$n_j v_{n_j} = 0$$

So, if there are no electrons  
there is no flux of electrons

(ii)

using the definition of the Avg. Velocity we have above i.e eq-①

we can say eventually that why a Band i.e completely filled with electrons is unable to contribute to the current?

So do we go wrong?

(High) High ... Hattaa

నుండి కొన్ని పాటు...!!

Q: The reason is when we integrate the integral over ' $k$ ', we are integrating over the Brillouin zone. The zone is symmetric with respect to origin of ' $k$ ' space.

So, let's take Integral in a special case where Band is completely filled with electrons.

కానీ ఈ ఫలితం ఏదు...!

i.e.  $\phi \equiv 1$  for the Band

$\phi$  is constant

Additionally it can be demonstrated that

$u(k)$  is odd i.e.

$$u(-k) = -u(k)$$

$\therefore$  The integral is zero.

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I wrote this as a speech to text format.

Prof. శ్రీ శ్రీ శ్రీ, దోష బుట్టి ఉండు.

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## Hole Average velocity

### Hole Average Velocity

$$J_{nj} = -qn_j v_{nj} = -q \int_{(j)} \mathbf{u}(\mathbf{k}) Q \Phi(\mathbf{r}, \mathbf{k}, t) d^3k.$$

Letting  $\Phi = 1 - (1 - \Phi)$  one gets

$$J_{nj} = q \int_{(j)} \mathbf{u} Q (1 - \Phi) d^3k - q \int_{(j)} \mathbf{u} Q d^3k,$$

where the second integral vanishes. As a consequence,

As we have seen

$$J_{nj} = -q n_j v_{nj} = -q \int_{(j)} \mathbf{u}(\mathbf{k}) Q \Phi(\mathbf{r}, \mathbf{k}, t) d^3k$$

This is the equation of electron current density which we derived above

→ Now by using a simple Mathematical trick we describe the concentration of holes as

$$\text{letting } \phi = 1 - (1 - \Phi)$$

Now

$$J_{nj} = q \int_{(j)} \mathbf{u} Q (1 - \phi) d^3k - q \int_{(j)} \mathbf{u} Q d^3k$$

Ans:- simple because  $\phi = 0$  ~~when  $\mathbf{r} = \mathbf{k}$~~   $\phi = 0$

This integral vanishes why?

This whole equation is an alternate way of saying that the state ' $j$ ' is filled with a hole or i.e absence of Electron

Because, we have the probability of electron as  $(1-\phi)$

$\phi$  : probability of presence of  $e^-$

$1-\phi$  : probability of absence of  $e^-$   
presence of Hole

The alternate equation we derived above for absence of electron concentration can be used for any Band.

→ We know that

Concentration of Holes =

$$P_j^o = \int_{(j)} \Omega (1-\phi) d^3 k$$

2

Here we will use both equations ① and ②

to give the Hole Current Density as

The hole concentration is

$$p_j = \int_{(j)} Q (1 - \Phi) d^3 k,$$

whence, indicating the hole current density with  $\mathbf{J}_{pj}$ ,

$$\mathbf{J}_{pj} = \mathbf{J}_{nj} = q p_j \frac{\int_{(j)} u Q (1 - \Phi) d^3 k}{\int_{(j)} Q (1 - \Phi) d^3 k} = q p_j v_{pj}$$

This is equivalent  
↑ to  $V_{pj}$

i.e.  $J_{pj} = J_{nj} = q p_j$

$$\int_j u Q (1 - \Phi) d^3 k$$

$$\int_j Q (1 - \Phi) d^3 k$$

This is equivalent to  $p_j$

Here, we multiplied and divided the eq'

$$q \int_j u Q (1 - \Phi) d^3 k \quad \text{with } p_j$$

∴ we can see that

$$J_{pj} = J_{nj} = q p_j V_{pj}$$

$q$ : Charge of Hole  $= +1.602 \times 10^{-19} C$

$p_j$ : Concentration of Holes

$v_{pj}$ : Avg. Velocity of Holes  $\Leftrightarrow$  Ratio of Integrals i.e.  $\frac{\int_{(j)} u Q (1 - \Phi) d^3 k}{\int_{(j)} Q (1 - \Phi) d^3 k}$



### Hole Average Velocity

$$\mathbf{J}_{nj} = -q n_j \mathbf{v}_{nj} = -q \int_{(j)} \mathbf{u}(\mathbf{k}) Q \Phi(\mathbf{r}, \mathbf{k}, t) d^3 k.$$

Letting  $\Phi = 1 - (1 - \Phi)$  one gets

$$\mathbf{J}_{nj} = q \int_{(j)} \mathbf{u} Q (1 - \Phi) d^3 k - q \int_{(j)} \mathbf{u} Q d^3 k,$$

where the second integral vanishes. As a consequence,

- The current density of the  $j$ th band may also be thought of as given by the motion of the empty states (holes), having the velocity  $\mathbf{u}(\mathbf{k})$  and the positive charge  $q$ .

The hole concentration is

$$p_j = \int_{(j)} Q (1 - \Phi) d^3 k,$$

whence, indicating the hole current density with  $\mathbf{J}_{pj}$ ,

$$\boxed{\mathbf{J}_{pj} = \mathbf{J}_{nj} = q p_j \frac{\int_{(j)} \mathbf{u} Q (1 - \Phi) d^3 k}{\int_{(j)} Q (1 - \Phi) d^3 k} \doteq q p_j \mathbf{v}_{pj}}$$

- The charge density due to the holes of the  $j$ th band is  $\rho_{pj} = qp_j$ ,  $q = 1.602 \times 10^{-19}$  C. The current density is  $\mathbf{J}_{pj} = \rho_{pj} \mathbf{v}_{pj} = qp_j \mathbf{v}_{pj}$ . The current density of a band 'j' with holes.

They care  
kind of  
self respiratory  
we use the  
eqn of electrons  
to derive  
Hole Avg. Velocity

→ we could either use electrons or holes to describe the population, current density of any band in practice what is done is .

For conduction Band: We prefer description using electrons

For Valence Band: We prefer description using holes.

The reason is in C.B The electrons stay near to the bottom (i.e minima) of the band.

∴ it legitimate to use parabolic Band Approximation.

Similarly, in V-B The holes stay near the Maxima of the Band ∴ we can use parabolic Band Approximation to describe the dynamics of the particle

### Dynamics in the Parabolic-Band Approx. — I

Taking a wave packet near the  $a$ th minimum of the conduction band, the diagonal expansion of  $E(\mathbf{k}) = E_n(\mathbf{k})$  yields

$$E(\mathbf{k}_0) \simeq E_C + \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (k_{i0} - k_{ia})^2 \geq E_C.$$

Letting  $E_e \doteq E(\mathbf{k}_0) - E_C \geq 0$ ,  $\delta k_i \doteq k_{i0} - k_{ia}$ ,

$$\hat{m}_a \doteq \begin{bmatrix} m_{1a} & 0 & 0 \\ 0 & m_{2a} & 0 \\ 0 & 0 & m_{3a} \end{bmatrix}, \quad \hat{m}_a^{-1} = \begin{bmatrix} m_{1a}^{-1} & 0 & 0 \\ 0 & m_{2a}^{-1} & 0 \\ 0 & 0 & m_{3a}^{-1} \end{bmatrix},$$

and indicating with  $1/\hat{m}_a$  the inverse mass tensor  $\hat{m}_a^{-1}$ , the expansion becomes

$$E_e \simeq \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} \delta k_i^2 = \hbar \delta \mathbf{k} \bullet \frac{1}{2\hat{m}_a} \hbar \delta \mathbf{k}.$$

As a consequence, the group velocity  $\mathbf{u}_g = \mathbf{u}_{ng}$  reads

$$\mathbf{u}_g = \frac{1}{\hbar} \text{grad}_{k_0} (E_e + E_C) = \frac{1}{\hat{m}_a} \hbar \delta \mathbf{k}.$$

“ ఈ కాదు విభిన్నమైలు, లేక ఇంకొను,,  
మాట్లాడును, నేర్చుతో నేర్చుకొవాలు ”

Dos and Energy bands

Starting

→ we studied about parabolic band approx. because it is convenient to describe the dynamics of particle.

In the conduction Band

$$E(k_0) \approx E_C + \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (k_{i0} - k_{ia})^2 \geq E_C$$

↓  
minimum  
of conduction  
Band

↓  
2nd order expansion  
of  $E(k_0)$

If we remember

we have also introduced the Effective Mass

That are the 3 coefficients  $m_{ia}$  introduce denominator and are related to the 2nd derivative of Energy function w.r.t  $k$

→ we already know  
 In a Semiconductor like Silicon when  
 we are in the vicinity of minimum of  
 Conduction Band then one of the elements  
 of effective masses  $m_{1a}$  is different  
the other two are equal to each other.

→ In this Stage we are distinguishing The  
 effective masses we are just giving them  
 names as show below.

$$\hat{m}_a = \begin{bmatrix} m_{1a} & 0 & 0 \\ 0 & m_{2a} & 0 \\ 0 & 0 & m_{3a} \end{bmatrix} = \text{Effective mass Tensor}$$

$a$ : counter of the minimum

$$m_a^{-1} = \begin{bmatrix} m_{1a}^{-1} & 0 & 0 \\ 0 & m_{2a}^{-1} & 0 \\ 0 & 0 & m_{3a}^{-1} \end{bmatrix}$$

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→ we arrange the effective masses in a Tensorform i.e Matrix, The matrix is diagonal because all the other second derivatives of the  $E$  wrt  $\mathbf{k}$  are zero

Q Why do we introduce Tensors?

Ans. Because, we want to express the expansion in a Tensor form. rather than Taylor's Expansion

$$E(\mathbf{k}_0) \simeq E_C + \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (k_{i0} - k_{ia})^2 \geq E_C.$$

Letting  $E_e \doteq E(\mathbf{k}_0) - E_C \geq 0$ ,  $\delta k_i \doteq k_{i0} - k_{ia}$ ,

$$\hat{m}_a \doteq \begin{bmatrix} m_{1a} & 0 & 0 \\ 0 & m_{2a} & 0 \\ 0 & 0 & m_{3a} \end{bmatrix}, \quad \hat{m}_a^{-1} = \begin{bmatrix} m_{1a}^{-1} & 0 & 0 \\ 0 & m_{2a}^{-1} & 0 \\ 0 & 0 & m_{3a}^{-1} \end{bmatrix},$$

and indicating with  $1/\hat{m}_a$  the inverse mass tensor  $\hat{m}_a^{-1}$ , the expansion becomes

$$E_e \simeq \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} \delta k_i^2 = \hbar \delta \mathbf{k} \bullet \frac{1}{2\hat{m}_a} \hbar \delta \mathbf{k}.$$

As a consequence, the group velocity  $\mathbf{u}_g = \mathbf{u}_{ng}$  reads

$$\mathbf{u}_g = \frac{1}{\hbar} \text{grad}_{k_0} (E_e + E_C) = \frac{1}{\hat{m}_a} \hbar \delta \mathbf{k}.$$

$$\underline{E(k_0) - E_C} \approx \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (k_{io} - k_{ia})^2$$

$\downarrow$

$$E_e \approx \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (k_{io} - k_{ia})^2$$

kinetic energy of the  
particle i.e electron

$$E_e \approx \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} (\delta k_i)^2 \quad \xrightarrow{\text{green arrow}} (k_{io} - k_{ia})^2$$

If we consider a vector notation where

the 3 components of  $\delta k_i$  to a

single column vector called  $\delta \mathbf{k}$

& then we introduce symbol of effective mass tensor we can rewrite the kinetic energy in this form.

$$E_e \approx \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_{ia}} \delta k_i^2 = \hbar \delta \mathbf{k} \cdot \frac{1}{2m_a} \hbar \delta \mathbf{k}.$$

$$E_e = \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_i a} (f_k)^2 = \hbar \delta k \cdot \frac{1}{\hat{m}_a} \hat{m}_a^{-1} \hbar \delta k$$

As a consequence,  $u_g = u_{ng}$  reads

$$u_g = \frac{1}{\hbar} \operatorname{grad}_{k_0} (E_e + E_c) = \frac{1}{\hat{m}_a} \hbar \delta k$$

Total  
Energy  
i.e  $E(k_0)$

$$u_g = \hat{m}_a^{-1} \hbar \delta k$$

$$\because E_e = \frac{1}{2} \sum_{i=1}^3 \frac{\hbar^2}{m_i a} f_k^2$$

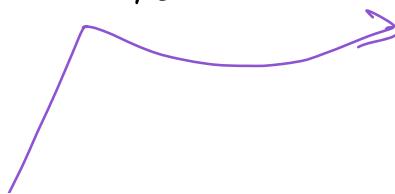
$$f_k^2$$

quadratic

$\therefore E_e$  is even  
function

$\therefore$  The derivative of an Even function is odd  
we have

$$u_g = \frac{1}{\hbar} \operatorname{grad}_{k_0} (E_e + E_c) = \frac{1}{\hat{m}_a} \hbar \delta k$$



odd function

↙

→ This explains better why Groupvelocity  
is odd w.r.t  $\mathbf{k}$ .

### Dynamics in the Parabolic-Band Approx. — II

The work exerted onto the packet by an external force  $-\text{grad}_{r_0} U = \hbar \dot{\mathbf{k}}_0$  during the time  $dt$  is

$$\begin{aligned} dW &= \hbar \dot{\mathbf{k}}_0 \bullet d\mathbf{r}_0 = \hbar \dot{\mathbf{k}}_0 \bullet \mathbf{u}_g dt = \hbar \delta \dot{\mathbf{k}} \bullet \frac{1}{m_a} \hbar \delta \mathbf{k} dt = \\ &= \frac{d}{dt} \left( \hbar \delta \mathbf{k} \bullet \frac{1}{2m_a} \hbar \delta \mathbf{k} \right) dt = dE_e. \end{aligned}$$

This shows that  $E_e$  is the kinetic energy of a wave packet near the  $a$ th minimum of the conduction band. As the states near  $E_C$  are occupied by electrons, it is  $U = U_c = -q\varphi_e$ , where  $\varphi_e$  is the electric potential acting on them; whence  $\hbar \delta \dot{\mathbf{k}} = -\text{grad} U_e = q \text{grad} \varphi_e = -q \mathcal{E}_e$ , with  $\mathcal{E}_e$  an electric field. More generally it can be shown that, if a magnetic field is also acting on the electron,  $\hbar \delta \dot{\mathbf{k}}$  is given by the Lorentz force

$$\hbar \delta \dot{\mathbf{k}} = \mathbf{F}_e = -q (\mathcal{E}_e + \mathbf{u}_g \wedge \mathbf{B}).$$

This description of the dynamics holds as long as the electron does not undergo a collision. If a collision occurs, the force during the collision is very strong and  $U$  cannot be treated any more as a perturbation superimposed on  $V$ .

~~If we~~ we can also demonstrate that  $E_e$  is the kinetic energy of the electron - we can achieve this by applying General theorem of Mechanics.

The General Theorem tells us that

particle subjected to Force changes

K.E of particle :

→ This variation of K.E is equal to the work exerted by the external force onto that particle.

Q How do we define a work ?

The work exerted onto the packet by an external force  $-\text{grad}_{r_0} U = \hbar \dot{k}_0$  during the time  $dt$  is

$$dW = \hbar \dot{k}_0 \bullet dr_0 = \hbar \dot{k}_0 \bullet u_g dt = \hbar \delta \dot{k} \bullet \frac{1}{\hat{m}_a} \hbar \delta k dt = \\ = \frac{d}{dt} \left( \hbar \delta k \bullet \frac{1}{2\hat{m}_a} \hbar \delta k \right) dt = dE_e.$$

Elementary work is scalar product of  $dr_0$   
Force & Variation of space during which the force is active.

→ A Force we know is The variation of Momentum = product of  $\hbar \delta k$

$$\text{Force} = \frac{d(\hbar k)}{dt} = \hbar \frac{dk}{dt} = \hbar \dot{k}$$

$$\therefore d\omega = \frac{\vec{F} \cdot \vec{v}_o}{\text{Force}} \cdot \frac{d\vec{r}_o}{\text{displacement}}$$

displacement  
(variation in space) =  $d\vec{r}_o = \frac{u_g dt}{\text{Velocity} \times \text{time}}$

Here we are considering single particle.

$$d\omega = \vec{F} \cdot \vec{v}_o \cdot u_g dt = \vec{F} \cdot \left( \frac{1}{m_a} \vec{F} dt \right)$$

$$d\omega = \frac{d}{dt} \left( \vec{F} \cdot \frac{1}{m_a} \vec{F} dt \right) \rightarrow F_e$$

$$d\omega = dE_e$$

Q What are the typical types of forces that act on electron?

Typically they are electric (or) electro magnetic forces.

If the force is purely electric and is derived from a potential energy

$$U = \underbrace{U_e}_{\substack{\downarrow \\ \text{potential} \\ \text{energy}}} = -q \underbrace{\phi_e}_{\substack{\downarrow \\ \text{electric} \\ \text{potential}}}$$

Hence  $\vec{F} = -\nabla U_e$

$$= q \nabla \phi_e$$

$$= q \vec{E}_e$$

If the force ~~is~~ also has magnetic field

$$\hbar \vec{F} = -q \left( \underline{\mathcal{E}_0} + \vec{u}_g \wedge \vec{B} \right)$$

Electric field      Magnetic field

### Dynamics in the Parabolic-Band Approx. — III



For an electron within a crystal, the relation between force and acceleration is typically anisotropic. E.g., in the parabolic-band approximation it is

$$\dot{\vec{u}}_g = \frac{1}{\hat{m}_a} \hbar \delta \vec{k} = \frac{1}{\hat{m}_a} \vec{F}_e.$$

If the entries of the mass tensor are different, the acceleration is not parallel to the force. This is due to the fact that the crystal structure is embedded in the mass tensor through the function  $E_n(\vec{k})$ . Only if the branch  $E_n$  is isotropic the mass tensor becomes a scalar:  $\hat{m}_a = m_a \mathcal{I}$ . For an anisotropic branch the acceleration may still be parallel to  $\vec{F}_e$ : this happens when the force is parallel to one of the coordinate axes; e.g.,

$$\vec{F}_e = F_e \vec{i}_1 \implies \begin{cases} \dot{u}_{1g} = F_e / m_{1a} \\ \dot{u}_{2g} = 0 \\ \dot{u}_{3g} = 0 \end{cases}$$

In fact, the reference in the direct lattice has a special role, because it is the reciprocal of a reference in the  $\vec{k}$  space such that the expansion of  $E_n(\vec{k})$  is diagonal.

→ It is interesting to check what happens to the dynamics of electrons in a crystal.

If we remember that the expression of the force is  $\nabla F \cdot \vec{r}$ , but we also know that if we divide force by Mass we get acceleration.

$$\ddot{u}_g = \frac{1}{\hat{m}_a} \nabla F \cdot \vec{r} = \frac{1}{\hat{m}_a} F_e.$$

This is true

~ Even though we are using Tensors to describe the phenomenon of Dynamics of Electron.

i.e velocity of the individual Electron

→ we have also seen that Group Velocity

$$u_g = \frac{1}{\hbar} \operatorname{grad}_{k_0} (E_e + E_c) = \frac{1}{\hat{m}_a} \nabla F \cdot \vec{r}$$

$$u_g = \frac{1}{\hat{m}_a} k \delta F$$

The time derivative of  $u_g$

$$\dot{u}_g = \frac{1}{\hat{m}_a} k \delta \dot{F} = \frac{1}{\hat{m}_a} F_e$$

Acceleration  
of  
electron

$$\Rightarrow F_e = \hat{m}_a \dot{u}_g$$

This is similar Newton's law of Acceleration.

Q What is the difference b/w Equations of Forces in Free Space & a Crystal?

A In Free space Mass is a scalar

Quantity i-e some constant

In a Crystal the Mass is a TENSOR.

We see immediately

If the entries of the mass tensor are different, the acceleration is not parallel to the force. This is due to the fact that the crystal structure is embedded in the mass tensor through the function  $E_n(\mathbf{k})$ . Only if the branch  $E_n$  is isotropic the mass tensor becomes a scalar:  $\hat{m}_a = m_a \mathcal{I}$ . For an anisotropic branch the acceleration may still be parallel to  $\mathbf{F}_e$ : this happens when the force is parallel to one of the coordinate axes; e.g.,

$$\mathbf{F}_e = F_e \mathbf{i}_1 \implies \begin{cases} \dot{u}_{1g} = F_e / m_{1a} \\ \dot{u}_{2g} = 0 \\ \dot{u}_{3g} = 0 \end{cases}$$

In fact, the reference in the direct lattice has a special role, because it is the reciprocal of a reference in the  $\mathbf{k}$  space such that the expansion of  $E_n(\mathbf{k})$  is diagonal.

→ The Mass Tensor derives from the presence of atoms where as the Force i-e applied as an Electric Field is a part of the total force that acts on an electron.

The Total Force that acts on an electron is the sum of The externally applied force, plus the action of all atoms on the electron.

→ The mass interaction equation represents the Mass Tensor which is dependent on the distribution of atoms in the crystal, which is different for Si, Ge, GaAs.

→ This is why when we apply External Force to the electron the Acceleration is not parallel to Force.

→ On the other hand, there are cases when acceleration is parallel to the Force.

$$\overline{3\text{H}\downarrow} \quad \overline{2\text{H}\downarrow} \quad \overline{\text{2m1H}\downarrow} \quad \overline{\text{4}\downarrow} \quad \overline{3\text{H}\downarrow}$$

~~But~~ Force ~~isn't~~  $\neq$  !

Crystal ~~and~~  $\neq$  Reaction of  
particle ~~and~~  $\neq$  !

→ If we remember in Gallium Arsenide GaAs there is only one minimum of the conduction Band and it's Isotropic. i.e. The equal Energy surfaces are straight fields.

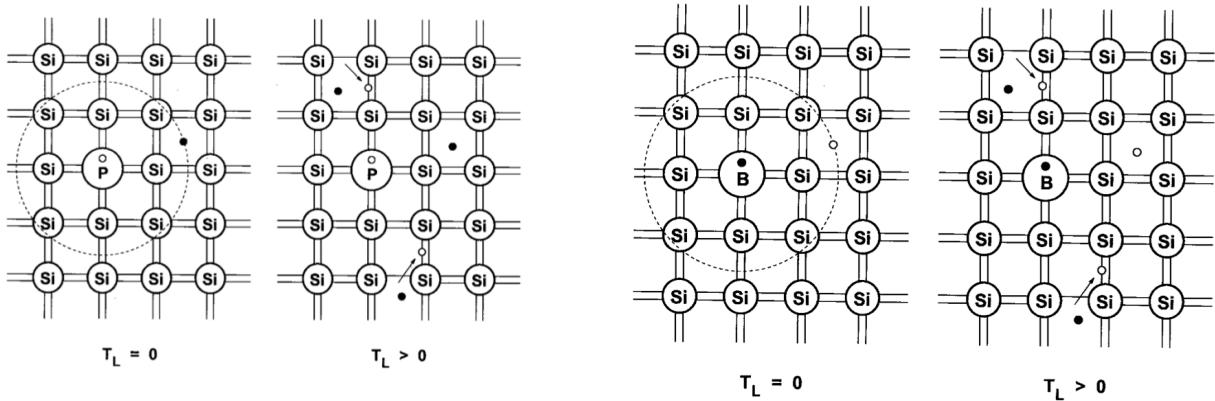
In this case for the Isotropic situation, the Mass tensor becomes

Scalar : a scalar:  $\hat{m}_a = m_a \mathcal{I}$ . For an anisotropic branch the acceleration may still be parallel to  $\mathbf{F}_e$ : this happens when the force is parallel to one of the coordinate axes; e.g.,

$$\mathbf{F}_e = F_e \mathbf{i}_1 \implies \begin{cases} \dot{u}_{1g} = F_e/m_{1a} \\ \dot{u}_{2g} = 0 \\ \dot{u}_{3g} = 0 \end{cases}$$

In fact, the reference in the direct lattice has a special role, because it is the reciprocal of a reference in the  $\mathbf{k}$  space such that the expansion of  $E_n(\mathbf{k})$  is diagonal.

Now we must start talking about Impurities in the Technology of Semiconductors. The Intrinsic Semiconductor is seldom used.



→ The impurities we introduce are called Dopants.

→ We introduce Dopants to improve conductivity of material & also we want to control the dependence of the conductivity on Temperature.

Phosphorus (V) Pentavalent  $\rightarrow$  n-type Semiconductor

Boron (III) Trivalent  $\rightarrow$  p-type Semiconductor

$\rightarrow$  When we are introducing Dopeants we are not forming a chemical compound

The no. of impurities we introduce is way less than the order of original silicon lattice.

$\rightarrow$  When pentavalent phosphorous (P) is introduced into silicon the P form four covalent bonds with adjacent silicon and the extra electron in the phosphorous atom becomes free electron in the crystal for a small amount of Energy.

→ ∴ as Temp ↑ the 5<sup>th</sup> electron in phosphorous atom becomes free

However, the distribution of Electric potential into vicinity of phosphorous atoms is such that there will be no Tunnel effect as we described earlier for silicon.

→ So the 5<sup>th</sup> electron now will be a free electron and it will able to provide current inside a Crystal.

→ The +ve charge inside the Phosphorous atom cannot move it will stay in the position of phosphorous atom.

i.e phosphorus will be ionized.

& it's an uncompensated +ve charge that will be fixed in the position of

phosphorous atom.

→ In parallel to this if we have increased the temperature some of the electrons belonging to silicon atom will get free as we have seen in pure silicon crystal and in that case **Electron-Hole pairs** will be created. The holes will be moving around with **TUNNEL EFFECT** as we described in Pure Silicon Crystal.

→ So, **Electrons** in the **Conduction Band** provided by both **silicon & phosphorous atoms** and **Holes** in the **(VB)** that will be provided <sup>only</sup> by **silicon atoms**, plus some fixed free charges attached to phosphorous atoms.

→ The issue is that at Room Temperature Intrinsic concentration of electrons in Silicon is in the range of  $\approx 10^{10}$  exactly ( $1.6 \times 10^9$ )

→ If we introduce into Si crystal the phosphorous atoms @  $10^{15}/\text{cm}^3$  it will be found that at Room Temp. all these phosphorous atoms will Ionize and contribute  $10^{15}$  electrons more which is 5 orders of magnitude more than Intrinsic concentration. So it is easily understood that <sup>with</sup> introduction of Dopeants we can control conductivity of the Material.

This is what happens in Space.  
we can repeat the analysis in Energies.

T. 23.2: Concentrazione dei portatori in un semiconduttore drogato di tipo n.



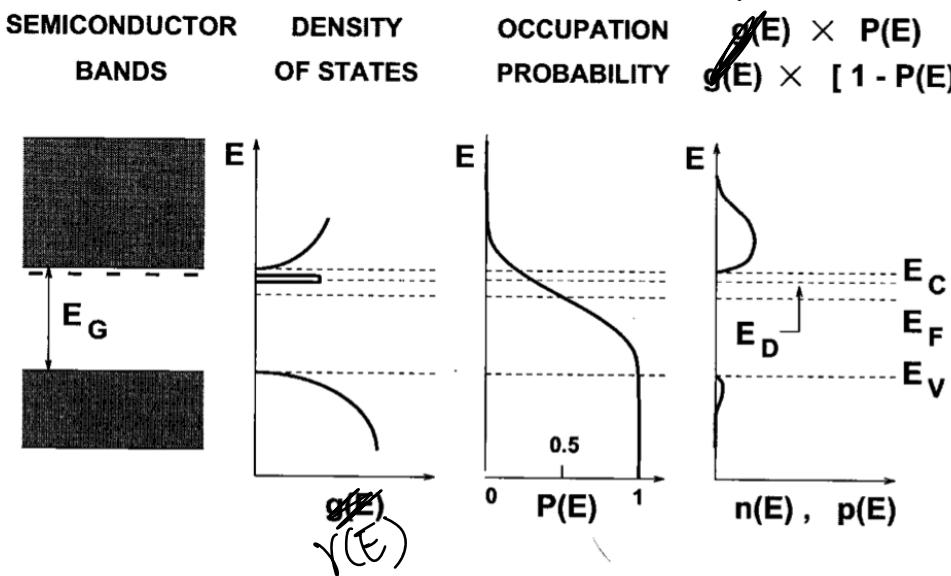
## DONOR-TYPE DOPING

(n-type semiconductor)

phosphorous

$$f(E)$$

$$\begin{aligned} & f(E) \times P(E) \\ & f(E) \times [1 - P(E)] \end{aligned}$$



→ We should ask one immediate question.



What happens to the structure of Bands with the Introduction of Dopants?



The Reasoning is The no. of Dopant phosphorous atoms introduced is way less than the silicon Atoms.

The concentration of silicon atoms in a silicon crystal  $\Rightarrow 5 \times 10^{20} / \text{cm}^3$

If  $10^{15}$  ph atoms are introduced it is like

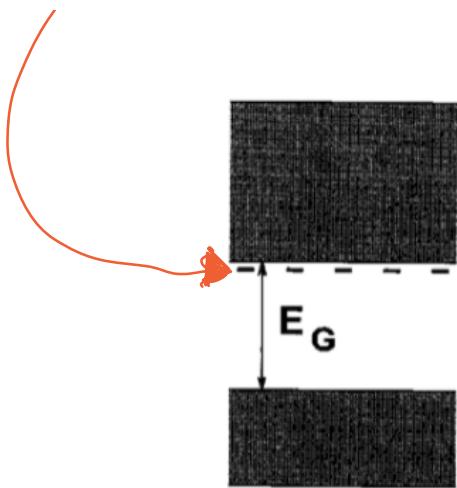
1 phosphorous atom  $\rightarrow$  10 million silicon atoms

\* However, ph atoms are impurities

These impurities add extra states

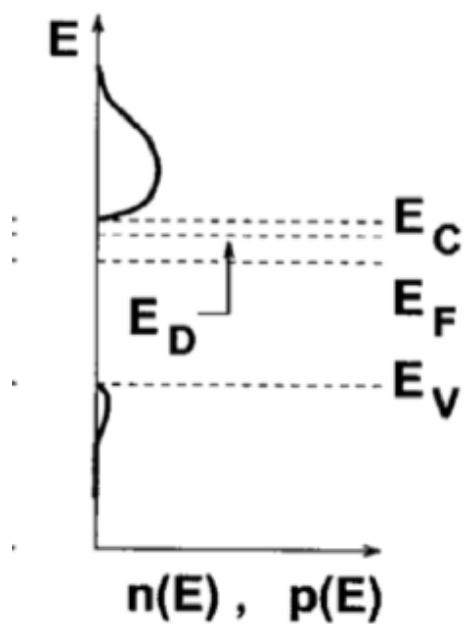
In particular ph atoms introduce states that are in the gap that are very near the edge of conduction Band - which is denoted by  $E_D$  and

Little Lines



Revanth Reddy Pannala  
EBIT, Unibo  
ప్రమాణ విషయ

$E_D$  : Energy states associated to the Dopant Ph



→ ' $E_D$ ' is just below the  $E_C$  because phosphorous Atom gives electron to CB with a slight amount of Energy

\* when we are at  $T = 0^\circ K$

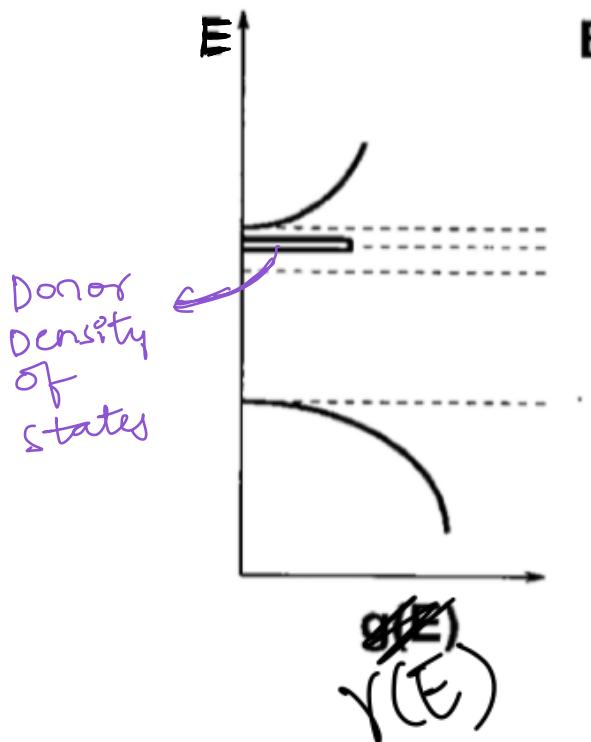
↗ All the states of Dopeart  $E_D$  are filled with one electron i.e attached to Ph atom.

When we go to Room Temperature we see that the Donor atoms that are so close to the Edge of the conduction Band that is easy for the Electron of the Donor states. To acquire Energy such that they go into the conduction Band.

The Distance b/w  $E_C$  &  $E_D$  can

be calculated and it is Approx.  $0.03 \text{ eV}$

## → DENSITY OF STATES



Here is the figure we can see that the Density of states is not affected against introduction of new Energy Bands by phosphorous atom.

Density of states is parabolic because we still use parabolic Band approximation

In the calculation of Density of states for Extrinsic Semiconductors the extra density of states because of Impurities is

indicated by Dirac Delta.

\* \* → If we assume that the Crystal is in Equilibrium we can assume that distribution of electrons in available states is the Fermi Statistics

\* \* However, The position of Fermi Level will not be in the middle of the Energy Gap. Because Now crystal is not intrinsic. The position of New Fermi Level should be calculated again with New situation based on the different Balance of charges in the Doped Semiconductor. We will do the calculation later.

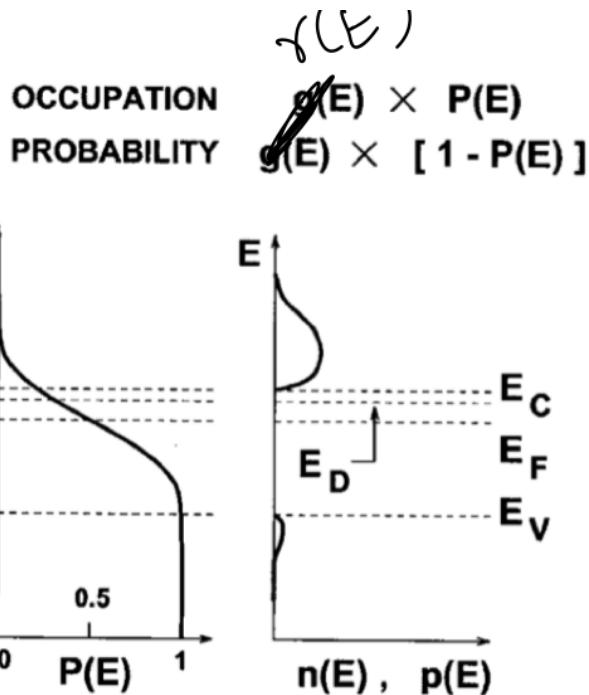
But, the Fermi Level instead of Being in the Middle of Energy Gap, will

move slightly upwards towards  
The Conduction Band ( $E_C$ )

i.e all the Fermi statistics will shift  
up for Extrinsic semiconductor.

As an obvious consequence, The  
probability of occupancy in CB will

Increases

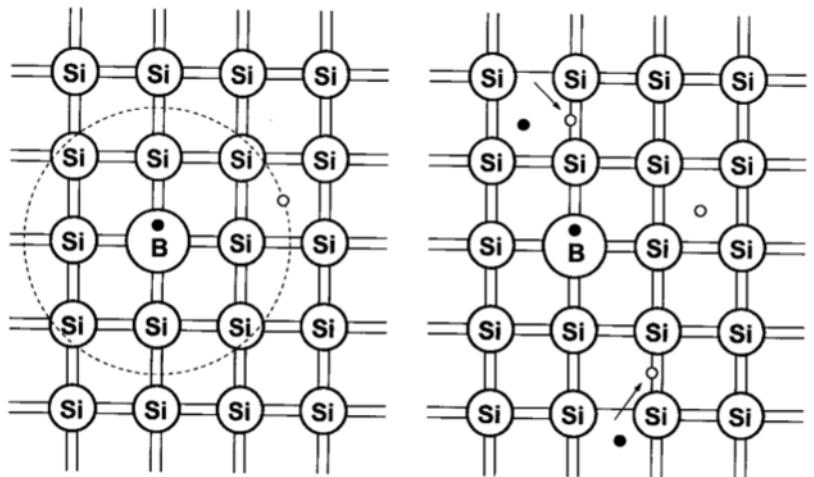


probability of occupancy of valence band decreases.

→ We can do the similar Analysis for the Trivalent Impurity **BORON**. because it belongs to 3rd column of Periodic Table

→ When, Boron is introduced as impurity it has only three electrons in the outer shell. So, 3 of these electrons will help in forming 3 covalent bonds with silicon but we have a missing Bond. In order to complete the Boron atom **Boron will create "Electron-Hole" pair** that will Borrow an electron from the crystal and form the **Fourth Bond**. But, in order to do so after acquiring one more electron  $\therefore$  the atom must be neutral. There must be Hole

compensating this electron - This hole orbits around BORON atom at  $0^{\circ}\text{K}$



At  $0^{\circ}\text{K}$

At Room Temperature

→ At Room Temperature of  $300^{\circ}\text{K}$

The Hole will become free, The electron will stay trapped with Boron atom and it cannot move.

So the free hole will be given to

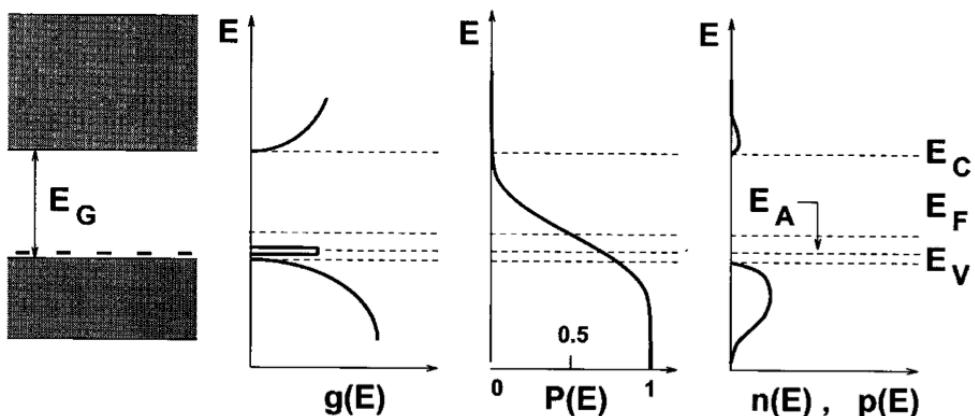
Valence Band at V.B will be Rich with holes.

→ There will be fixed -ve charges attached to the Boron atoms and in parallel Silicon atoms will provide in the generation of silicon and hole pairs.

## The Energy Band Diagram

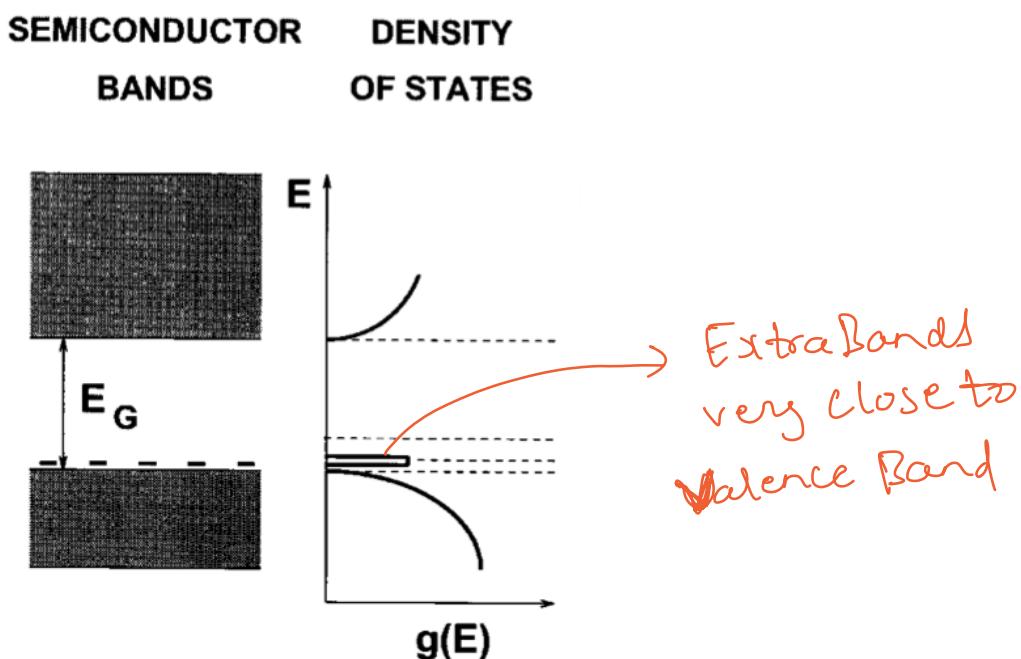
### ACCEPTOR-TYPE DOPING (p-type semiconductor)

SEMICONDUCTOR BANDS	DENSITY OF STATES	OCCUPATION PROBABILITY	$g(E) \times P(E)$	$g(E) \times [1 - P(E)]$
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The whole analysis is similar to that of n-type semiconductor.

→ Density of states of silicon is not disturbed with the introduction of Boron, but there will few new energy states that are introduced very close to the Valence Band.



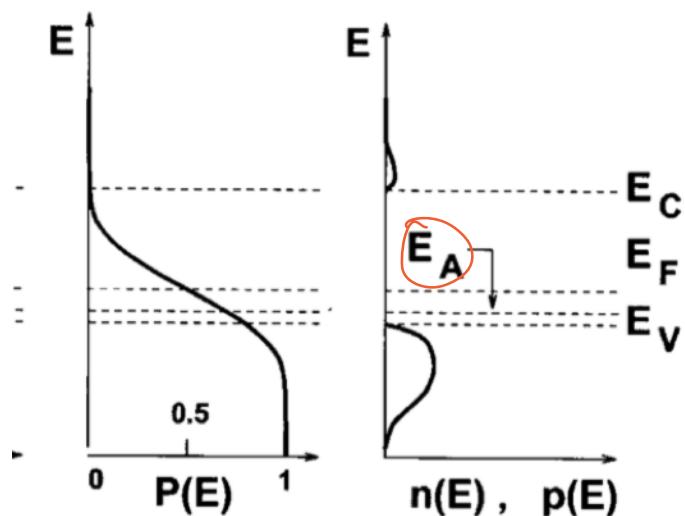
The Energy b/w New states and valence Band is very low 0.03 eV

∴ It would be easy for the New states to capture electrons from the

Valence Band and Introduce Holes  
in the V.B.

→ ∵ Boron accepts electrons it is called Acceptor Impurity & the New energy states are called Acceptor states.

$$\begin{array}{ll} \text{OCCUPATION} & f(E) \\ \text{PROBABILITY} & 1 - f(E) \times P(E) \\ & f(E) \times [1 - P(E)] \end{array}$$



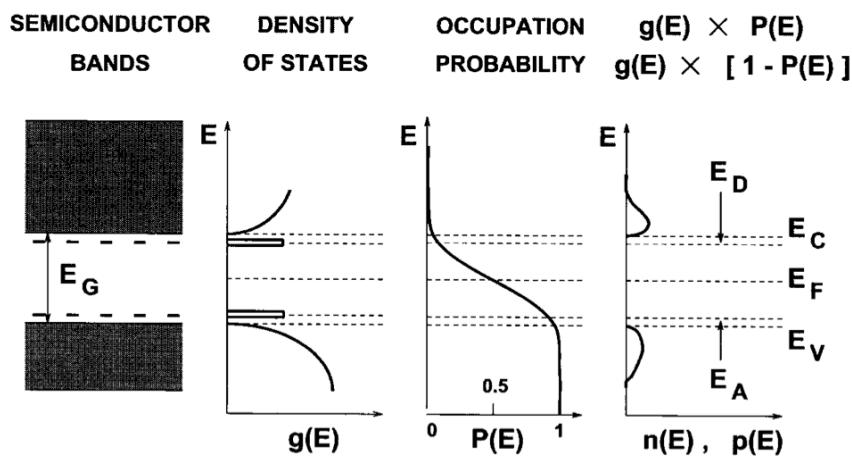
$E_A$ : Acceptor Energy state

→ The situation is Dual to that of n-type semiconductor.

# A Special Case

## DONOR- AND ACCEPTOR-TYPE DOPING

(compensated semiconductor)



CAP. 23: EFFETTI DOVUTI ALLE IMPUREZZE

T. 23.5: Concentrazione dei portatori in un semiconduttore compensato.

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T. 23.6: Espressioni usate nel calcolo della conc. estrinseca all'equilibrio (tipo n).

considering Equilibrium situation  
where we can use Fermi Statistics

only  
Donor atoms  
&  
Concentration  
of the Donor  
atoms is  
known.

### Extrinsic Concentration (n-Type) — I

Uniform doping ( $N_D = \text{const}$ ) — Equilibrium case

$$n \doteq N_c/\Omega = (1/\Omega) \int_{E_C}^{E_{CII}} g(E)P(E) dE \neq n_i$$

$$p \doteq N_h/\Omega = (1/\Omega) \int_{E_V}^{E_L} g(E)[1 - P(E)] dE \neq p_i$$

$$n_D \doteq (1/\Omega) \int_{\Delta E_D} g_D(E)P_D(E) dE = N_D - N_D^+$$

$$P(E) = \frac{1}{\exp[(E - E_F)/(k_B T_L)] + 1}, \quad E_F \neq E_{F_i}$$

$$\xi_c = -\frac{\zeta_c}{k_B T_L} = -\frac{E_C - E_F}{k_B T_L}, \quad \xi_h = -\frac{\zeta_h}{k_B T_L} = -\frac{E_F - E_V}{k_B T_L}$$

$$P_D(E) = \frac{1}{(1/d_D) \exp[(E - E_F)/(k_B T_L)] + 1}$$

$$g(E) \simeq \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \sqrt{E - E_C} \implies n = N_C \Phi_{1/2}(\xi_c)$$

$$g(E) \simeq \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} \sqrt{E_V - E} \implies p = N_V \Phi_{1/2}(\xi_h)$$

$$g_D(E) \simeq \Omega N_D \delta(E - E_D) \implies \begin{cases} n_D = N_D P_D(E_D) \\ N_D^+ = N_D [1 - P_D(E_D)] \end{cases}$$

→ Concentration of Densities is  $N_D$

\* if  $N_D$  is constant and known

then the material is uniform in space

so, it is still legitimate to calculate  
the total numbers and calculating  
concentration divided by the volume.

\* This is only possible if the material is  
uniform in space -

