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Electrons in Solids

Conduction in a band

i) There must be free electrons, i.e. no conduction in an empty C.B

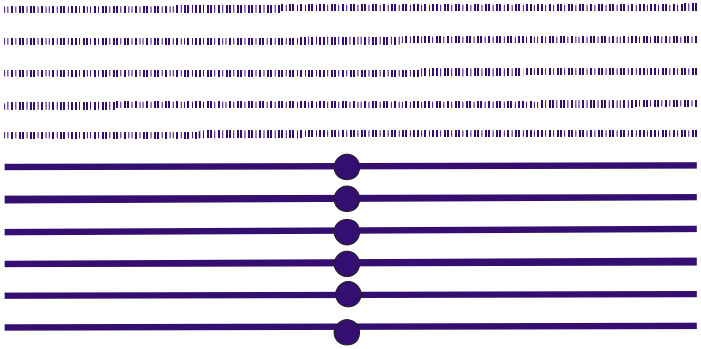
ii) There needs to be a band of states. If carriers gain energy there must be a higher empty level available, otherwise Paulis's exclusion principle violated.

Consequences:

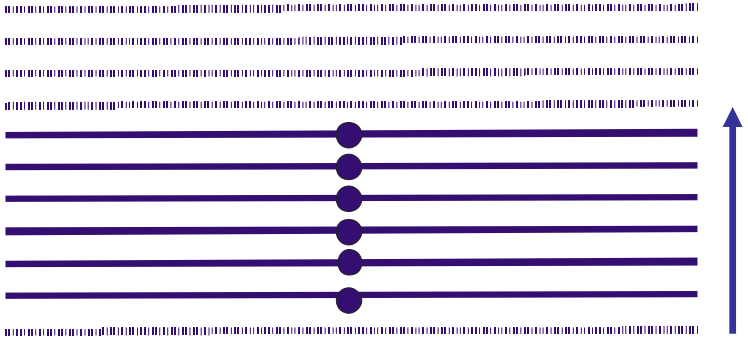
(a) an empty C.B. cannot support conduction

(b) a completely full band cant support conduction either

Band must be partially filled!



E-field =0



E-field >0

If electric field is applied, electrons gain energy and can move into higher energy empty states

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Electrons in Solids

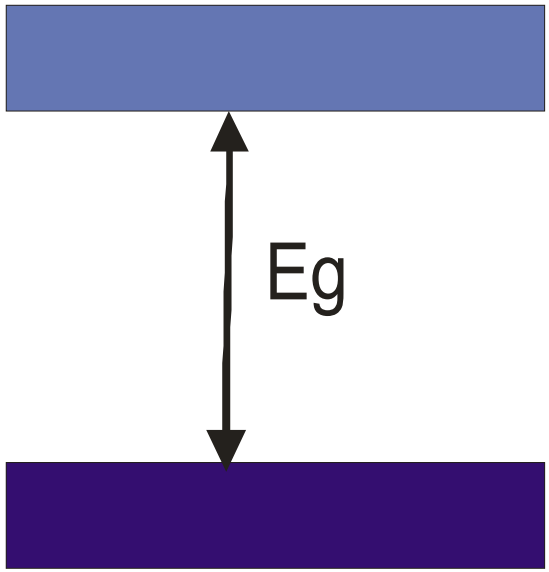
Insulators

Have a filled VB and a conduction band separated by a large energy gap (typically 5-20eV)

Only is electrons can acquire and energy E_g can they move into the CB.

Thermal energy = kT~ 0.025eV at 300K so probability is small

No (or very poor) conduction.



Metals

There electronic structure has a distinguishing feature.

Outer empty band overlaps the inner full band

As a result, you have a composite band and an ideal situation for conduction.

There is no energy gap. Electrons are free to move in an electric field to higher energy levels

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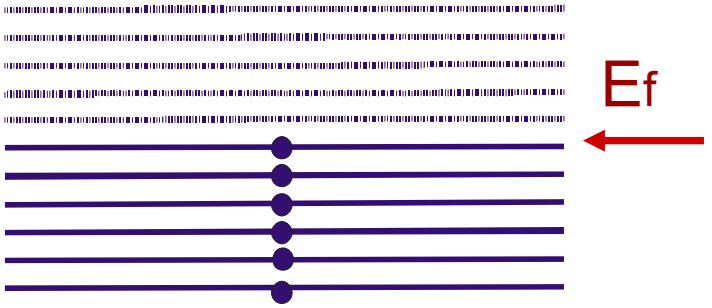
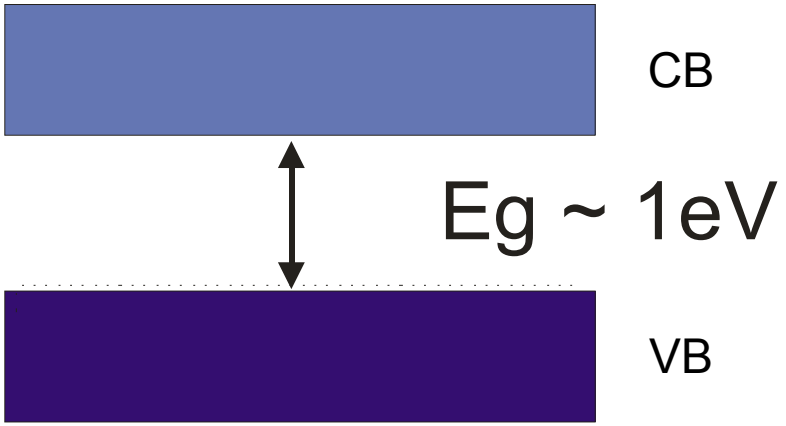
Electrons in Solids

We can define a fill level, known as the **FERMI LEVEL**

At OK, levels above the Fermi level are empty, levels below are full



In a **Semiconductor** the energy gap (Eg) ~ 1eV
At low temperature electrons cannot reach the CB: INSULATOR
Thermal energy = kT~ 0.025eV at 300K
So Eg> kT, but there is a now finite possibility of some electrons in the CB



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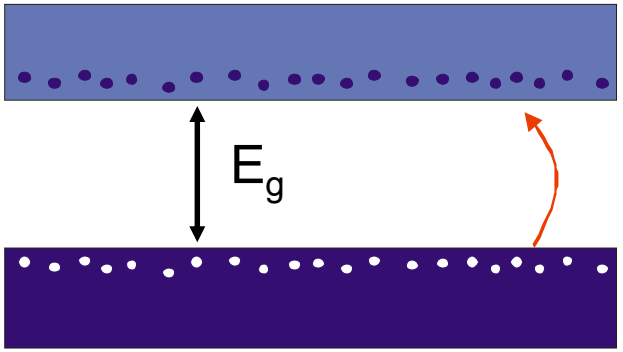
Electrons in Solids

Energy gap is sufficiently small that electrons can be promoted to the conduction band.



Each electron promoted to the CB leaves behind one vacant level (hole) in the VB. Conduction in semiconductors is due to:

(i) electrons moving in the part filled CB
(ii) electrons in the VB moving into levels vacated by electrons elevated into the CB. Easier to view as the movement of holes

In an intrinsic semiconductor:

number of electrons = n (m-3) = number of holes = p (m-3)
= n_i *(intrinsic concentration)*

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Energy bands& Occupation

Intrinsic Semiconductor

Know that **$n = p = n_i$.** Need n_i to determine the no. of electrons (holes) and then determine the conductivity (δ)

Since there are a large number of electrons (typ. $10^{28}m^{-3}$) in a semiconductor, we cant determine the conduction of every electron. However we can look at all the electrons statistically and determine the average behaviour of electrons

To help us, we define a probability distribution function called the

FERMI-DIRAC function) P(E)

Function P(E) gives the *probability* that an electron has an energy E (at some temperature T).
e.g. If $P(E_1)$ =0.2, 20% of electrons have $E = E_1$

The statistics that govern detailed form of P(E) depend on

1) type of particle
2) How these particles interact

If non interacting (e.g.: gas molecules) then they would be governed by Boltzmann statistics In this case the particles are electrons and are governed by Fermi-Dirac statistics i.e.: they must obey the Pauli exclusion principle

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Energy bands& Occupation

$$P(E) = \frac{1}{1 + e^{\frac{E - Ef}{kT}}}$$

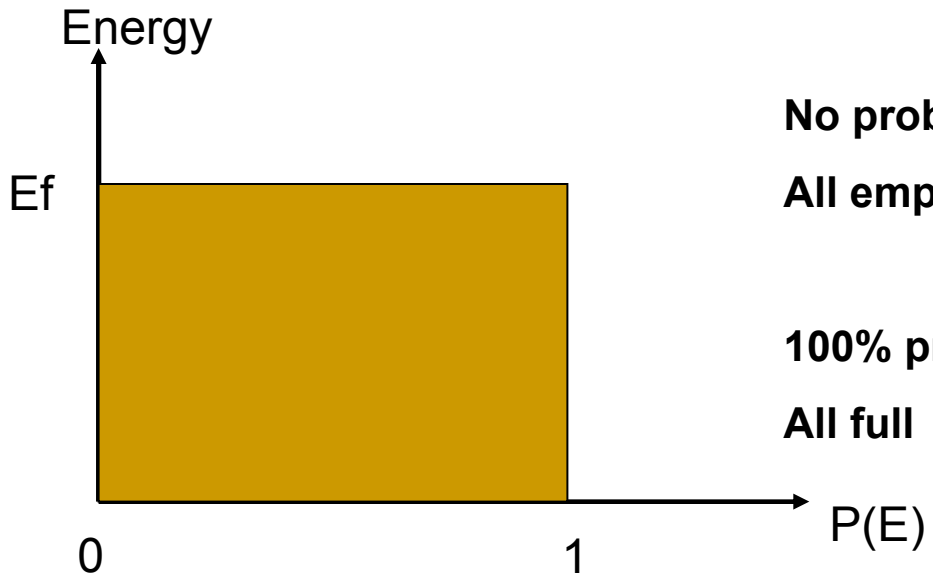
Where E_f is the Fermi level

P(E) is the probability that an electron has an energy E. P(E) varies from 0 to 1.

Two examples, at T=0K

E>E_f $P(E) = \frac{1}{1 + e^{\infty}} = 0$

E<Ef $P(E) = \frac{1}{1 + e^{-\infty}} = 1$



No probability for E>E_f

All empty

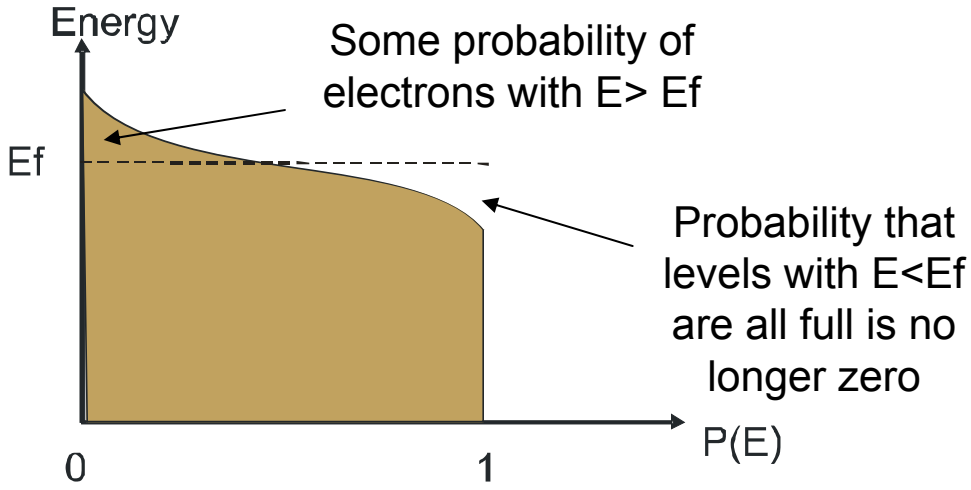
100% probability for E<E_f

All full

Energy bands& Occupation

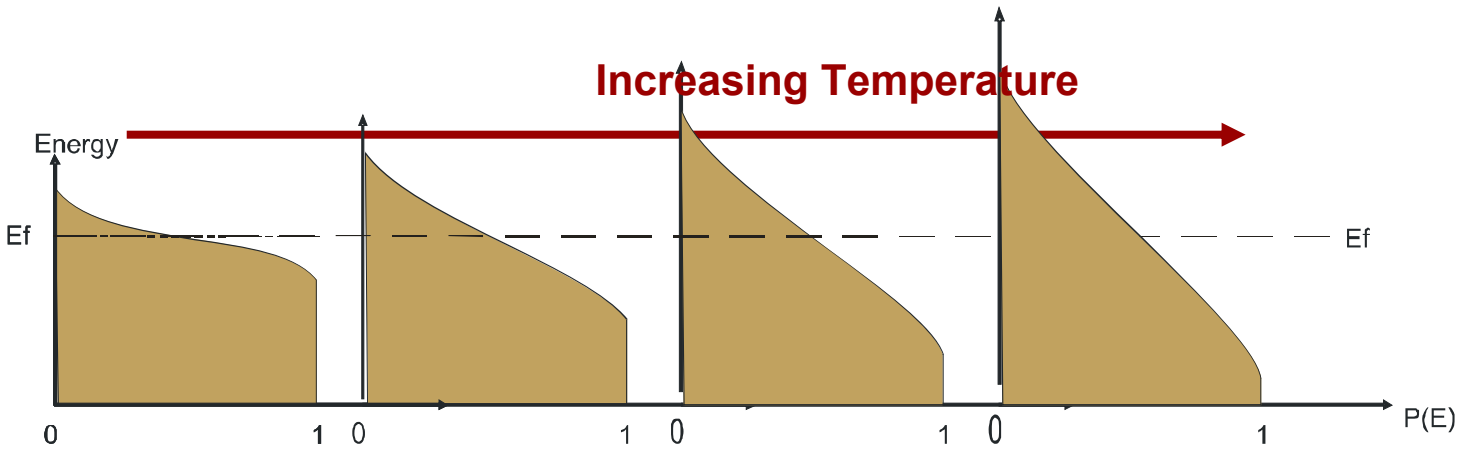
So what happens at higher temperature?

At T>0K there is always some possibility that electrons can have a higher energy than E_f. There probability will be higher the closer they are to E_f



Actual shape of P(E) depends on the function

As T increases the probability of E> E_f also increases, but P(E) is always symmetrical about E_f



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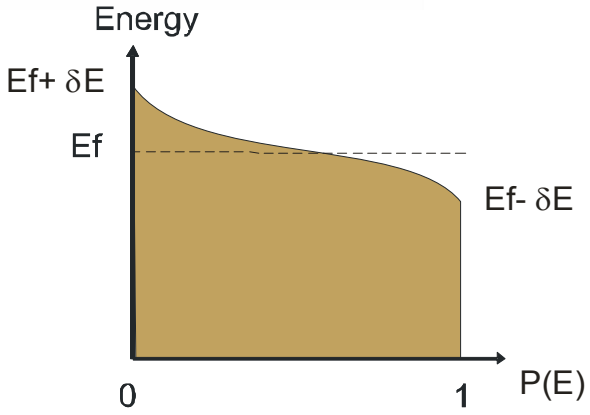
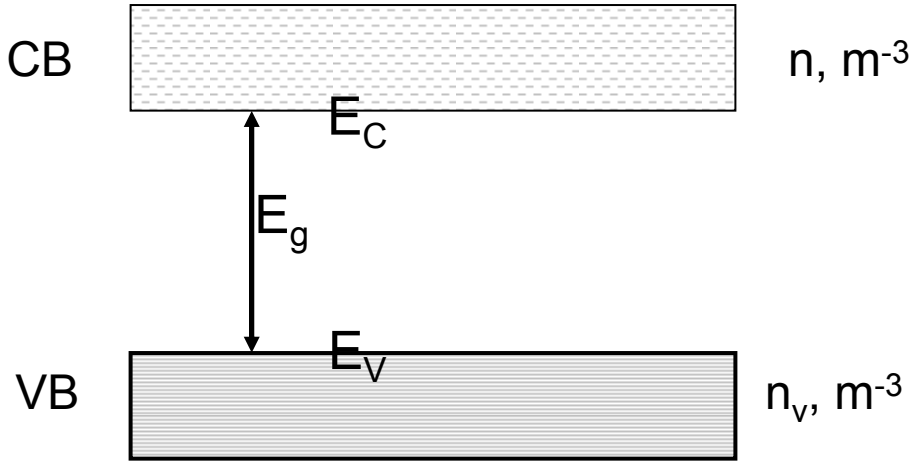
Energy bands& Occupation



$$P(E_f+\delta E) = 1-P(E_f-\delta E)$$



Apply to Semiconductor

Probability that an electron can gain enough energy to reach the CB is the probability that it can have energy E_v+E_g

Probability of an electron in the VB, energy E_v

$$P(E_v+E_g) = \frac{1}{1+e^{\frac{E_v+E_g-Ef}{kT}}}$$

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Energy bands& Occupation

If we assume n electrons in the CB at a temperature T and we have $n+n_v = n_{Tot}$ electrons in total, then

$n = n_{Tot} P(E_v + E_g)$

Probability of electrons in CB is:

$$n = \frac{n_{Tot}}{1 + e^{\frac{E_v + E_g - Ef}{kT}}}$$

Probability of electrons in VB is:

$$n_v = \frac{n_{Tot}}{1 + e^{\frac{E_v - Ef}{kT}}}$$

We know that $n_{Tot} = n + n_V$

$$n_{Total} = \frac{n_{Tot}}{1 + e^{\frac{E_v + E_g + E_f}{kT}}} + \frac{n_{Tot}}{1 + e^{\frac{E_v - Ef}{kT}}}$$

Solution is $E_f = E_g/2$.

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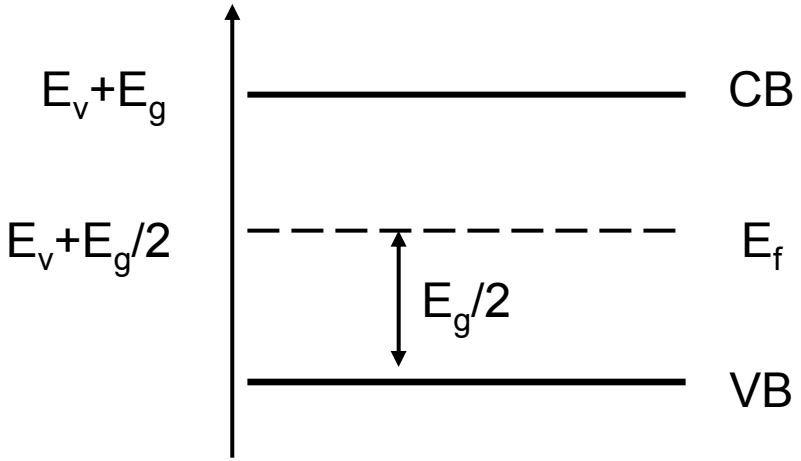
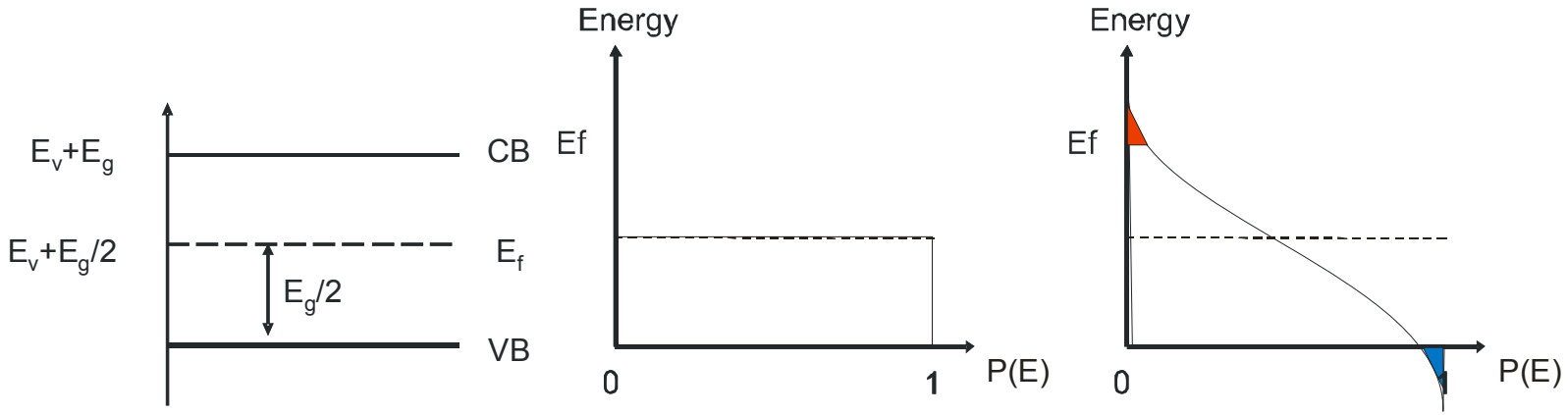
Energy bands & Occupation

In an INTRINSIC semiconductor, they Fermi level is mid way between the CB and the VB (mid gap)



As the temperature increases the probability that an electron occupies the CB increases. Always $n = p = n_i$, so we always have the same concentration of electrons as holes



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Energy bands & Occupation

$$n_i = \frac{n_{Tot}}{1 + e^{\frac{E_v + E_g - E_v - \frac{E_g}{2}}{kT}}}$$

$$n_i = \frac{n_{Tot}}{1 + e^{\frac{Eg}{2kT}}}$$

Semiconductors have different band gaps (E_g)

Material	Energy gap (eV)	
	0K	300K
Si	1.17	1.11
Ge	0.74	0.66
InSb	0.23	0.17
InAs	0.43	0.36
InP	1.42	1.27
GaP	2.32	2.25
GaAs	1.52	1.43
GaSb	0.81	0.68
CdSe	1.84	1.74
CdTe	1.61	1.44
ZnO	3.44	3.2
ZnS	3.91	3.6

As E_g increases, n_i decreases exponentially

$n_i \sim \exp(-E_g)$

As T increases, n_i increases exponentially
$n_i \sim \exp(-1/T)$

Need a 'useful' n_i, therefore useful E_g are in the range 0.1 to a few eV

Semiconductors are very temperature sensitive and device parameters can change a lot

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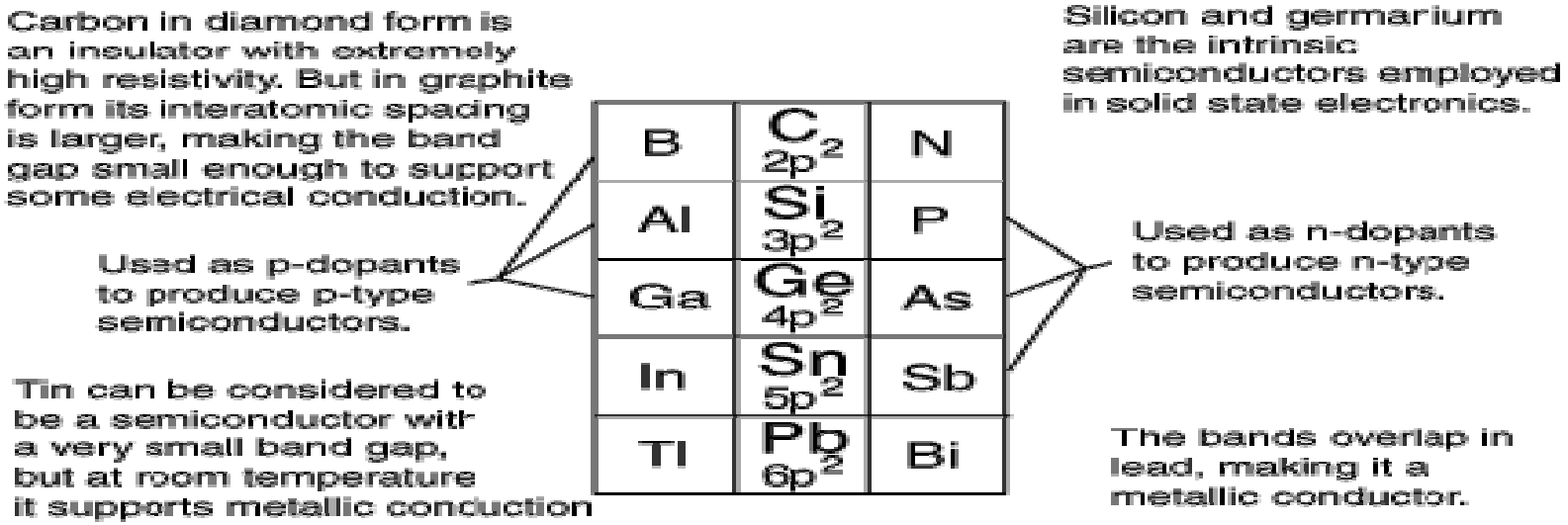
Energy bands & Occupation

Doped semiconductors

Intrinsic semiconductors are rarely used in practice since σ = F(Temp) only.

However we can vary the σ by using **doping** *(also known as extrinsic semiconductors)*



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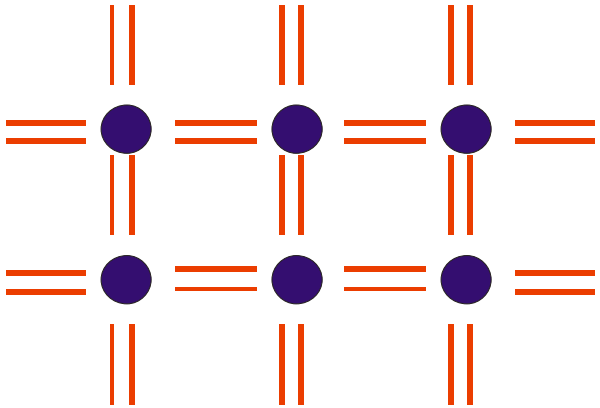
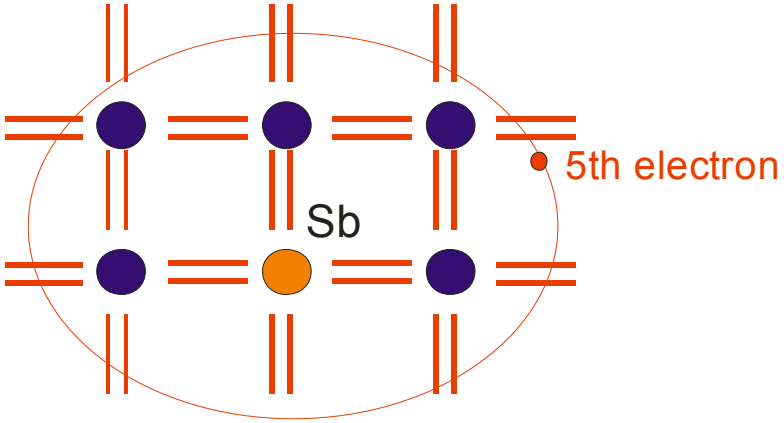
Energy bands & Occupation

n-type

Intrinsic (parent) material is Si. Has 4 electrons and 4 vacancies in the outer shell. Covalently bonded in diamond type structure.



We can add to the silicon n-type donors, such as phosphorus (P), arsenic (As), antimony (Sb), all have 5 electrons and 3 vacancies in outer shell. Dopant atoms substitute at Si site.



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Energy bands & Occupation

Only 4 electrons taken up as covalent bonds. The extra electron loosely bound to parent donor at 0K.

The extra electron behaves like a hydrogen (Bohr) atom except:

(i) Its mass (m_e) is different: $m_e \rightarrow m_e^*$

ii) $e_o \rightarrow e = e_o e_r$ since its orbit is in a dielectric e.g. Si

Hydrogen Bohr Model

$$E_i = \frac{me^4}{8\varepsilon_o^2 h^2 n^2} = \frac{13.6\ eV}{n^2}$$

$$E_i = \frac{13.6\ m_e^*}{\varepsilon_r^2 m}$$

For Si $\varepsilon r \sim 16$, $m_e^*/m = 0.6$

assume n=1

For Si, it predicts E_i = 0.03eV. Actually we observe 0.015eV

At most temperatures, $kT > \varepsilon_i$; (kT @ RT(300K) ~0.025 eV)

So at RT all donors are ionised (free, mobile). Each donor contributes 1 electron to C.B.

$n = N_d$ (the donor density)

But no extra holes produced in V.B, so not like intrinsic

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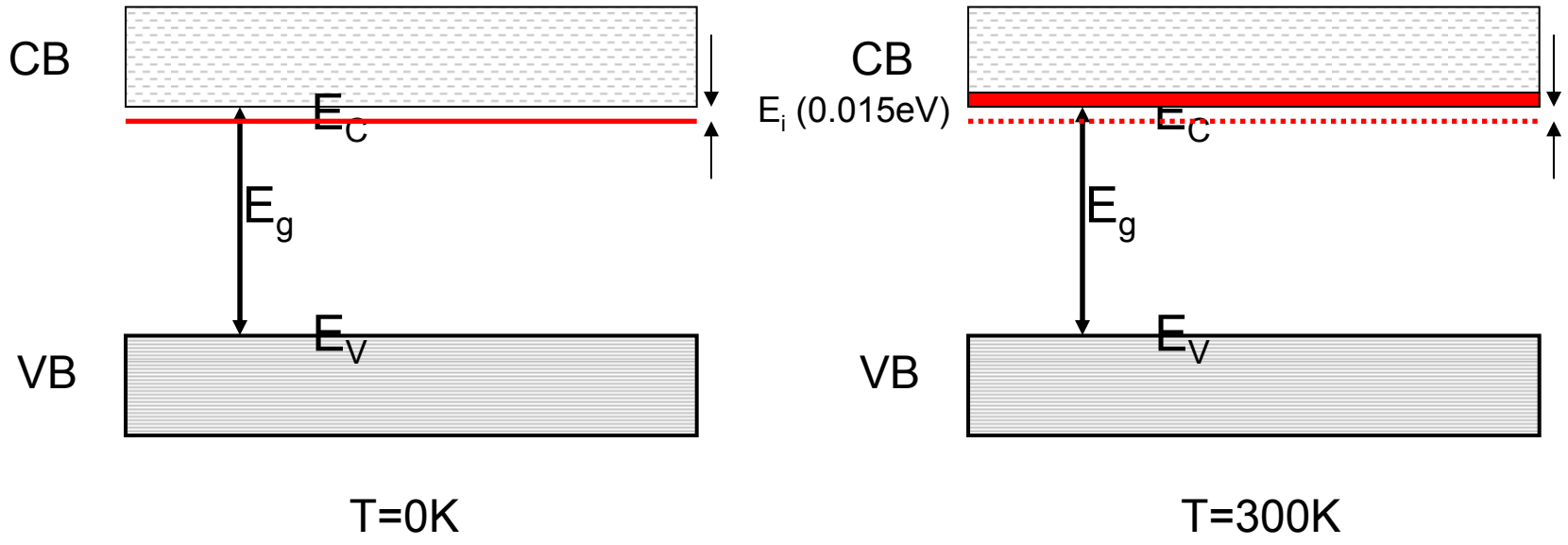
Energy bands & Occupation



So σ = *f*(Nd) $\neq$ *f*(T) provided all Nd's are ionised, e.g. at RT
Also small levels of dopant increase σ a lot.

e.g. intrinsic Si, ni = n = p = 10^{16} m^{-3} at RT

We can easily dope to higher levels than this

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Energy bands & Occupation

Dope the Silicon with 1 part in 10^6 with phosphorus donors. Si has 10^{28} atoms per m^3

$$N_d = \frac{10^{28}}{10^6} = 10^{22}\ m^{-3} = n$$

n = N_d, so

$$\frac{\sigma_n}{\sigma_i} \approx \frac{n}{n_i} = \frac{10^{22}}{10^{16}} = 10^6$$

One important rule for semiconductors, **$n\,p = n_i^2$**

$$p = \frac{n_i^2}{n} = \frac{(10^{16})^2}{10^{22}} = 10^{10} \ll p_i\ (= 10^{16})$$

Conductivity $\sigma = n_e m_e + p_e m_h$. Can ignore n_i and p in n-doped material

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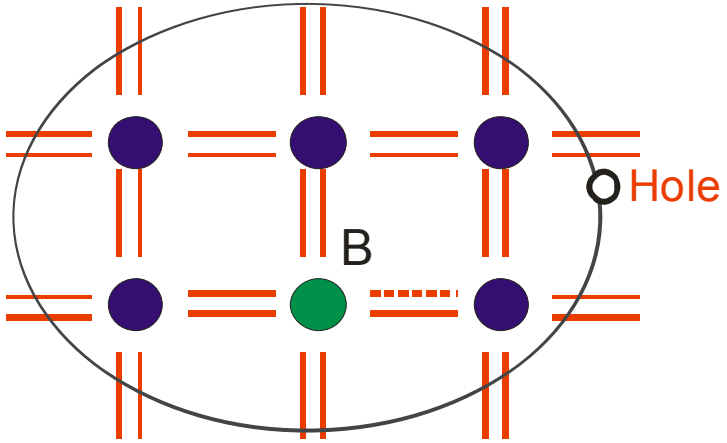
Energy bands & Occupation

p-type semiconductors

P-type dopants are called acceptors – 3 electrons and 5 vacancies in the outer shell, e.g. boron

Vacancy or hole– loosely bound to parent atom – an electron can move into vacancy and create a hole.

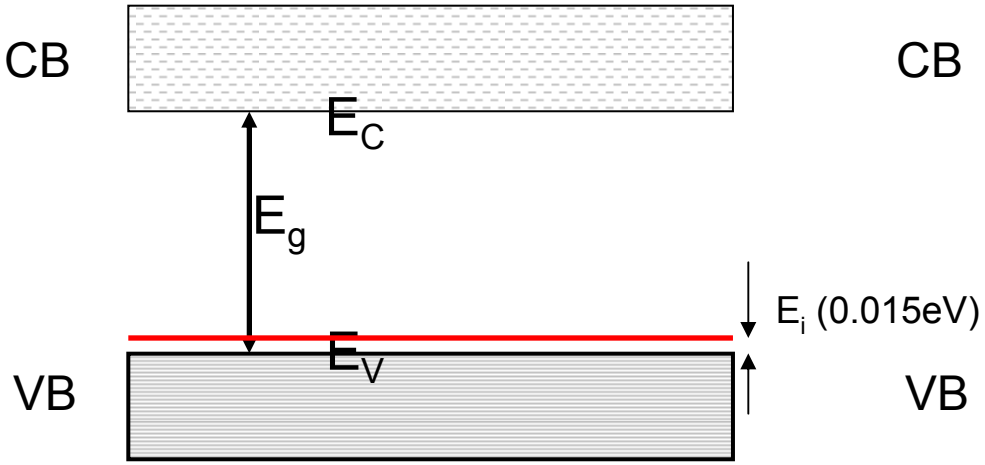
Energy needed again ~0.01eV.



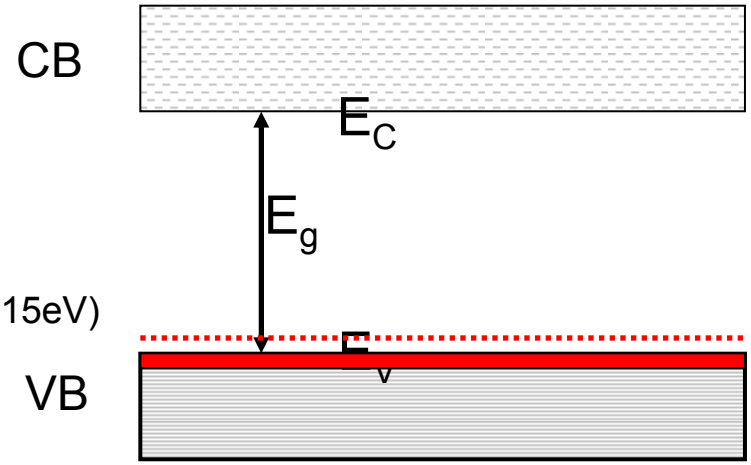
Every Boron atom produces 1 hole, i.e. N_a (acceptor density) = p (free holes.

$p = N_a >> pi.$ Again $n\,p = ni^2.$ $n << n_i.$

$\sigma p >> \sigma i$



T=0K



T=300K

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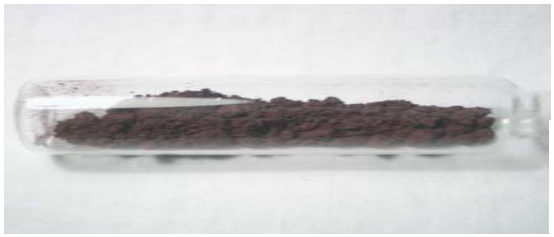
Making Doped Silicon

+



Silicon (few Kg)

Phosphorus (few μg)