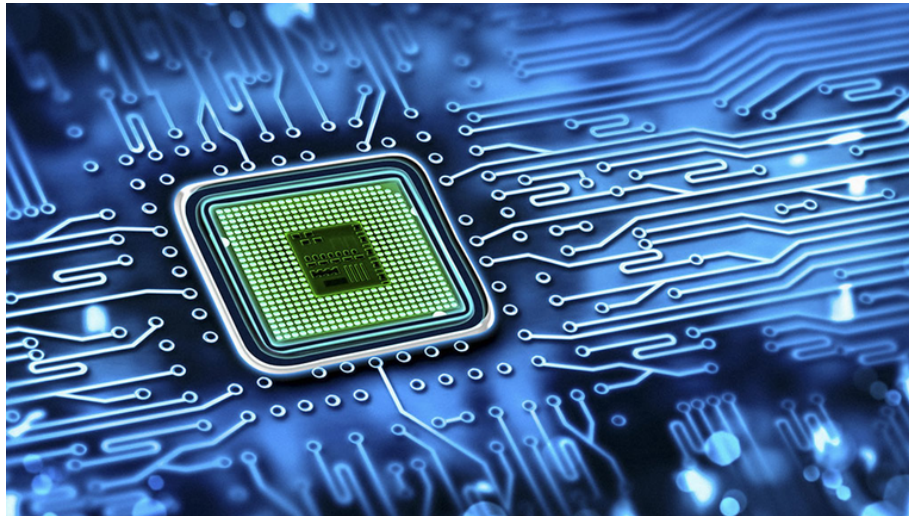
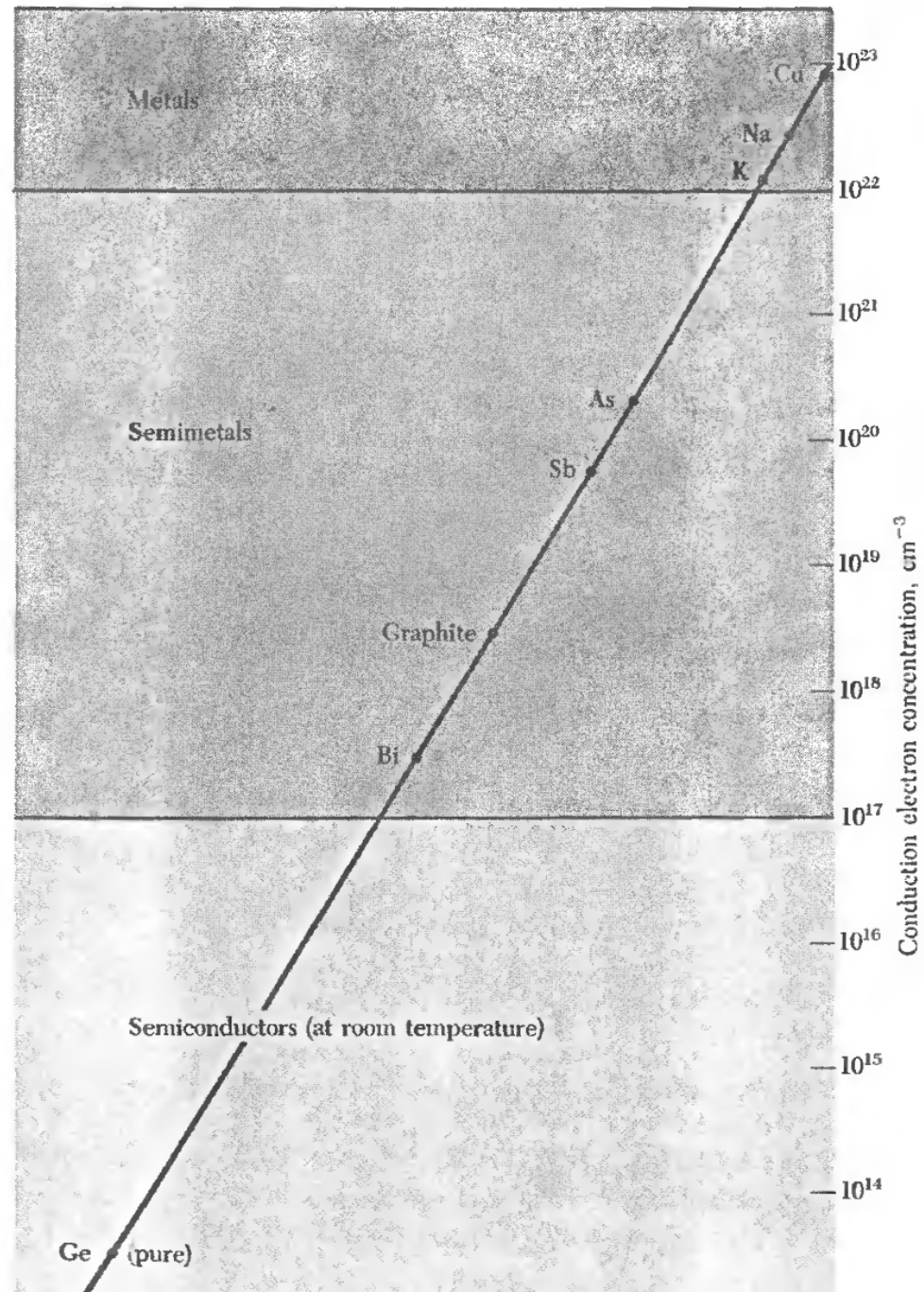


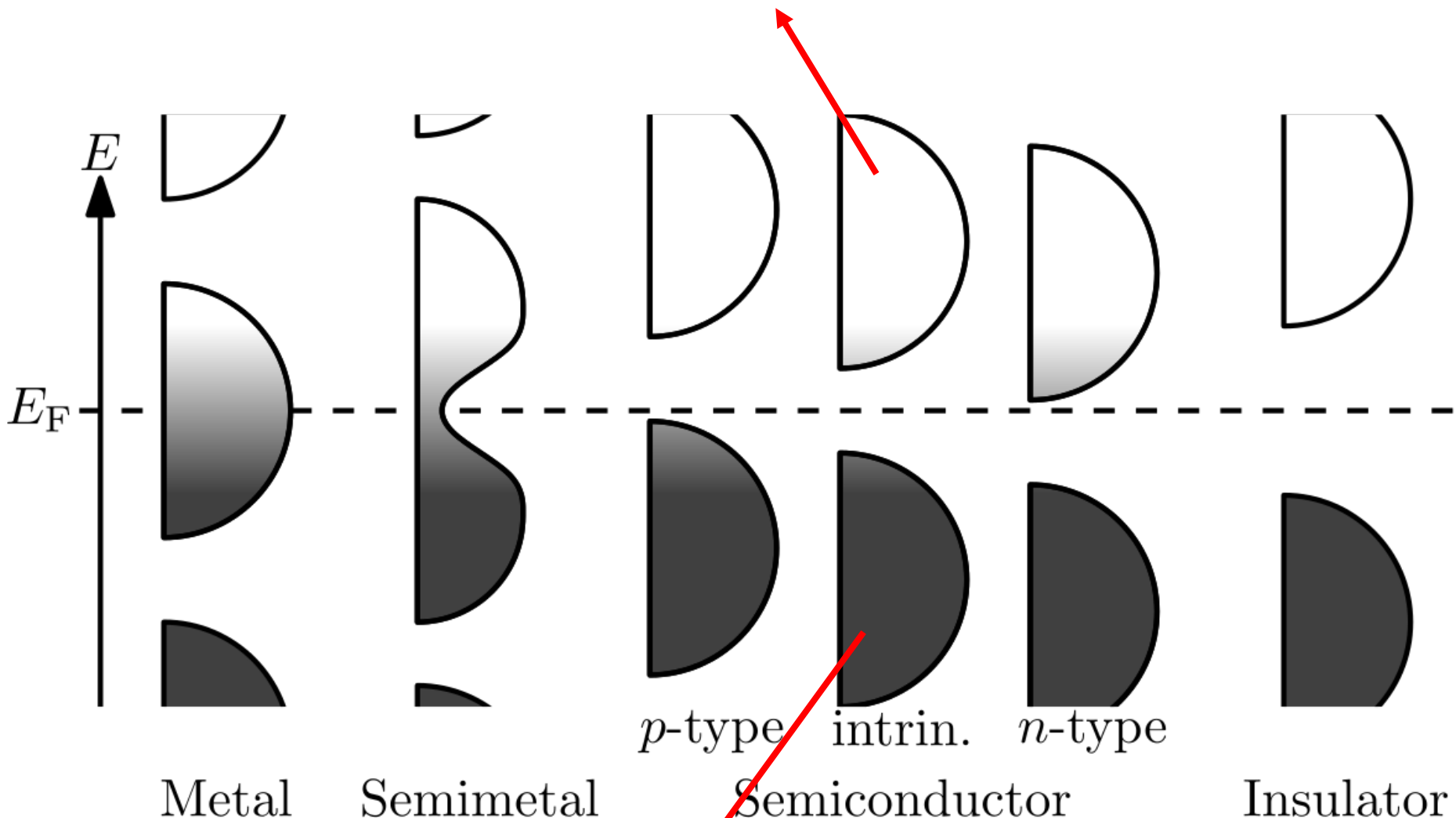
Capítulo 8: Semiconductores



Concentración de portadores que contribuyen a la conducción eléctrica en diferentes materiales



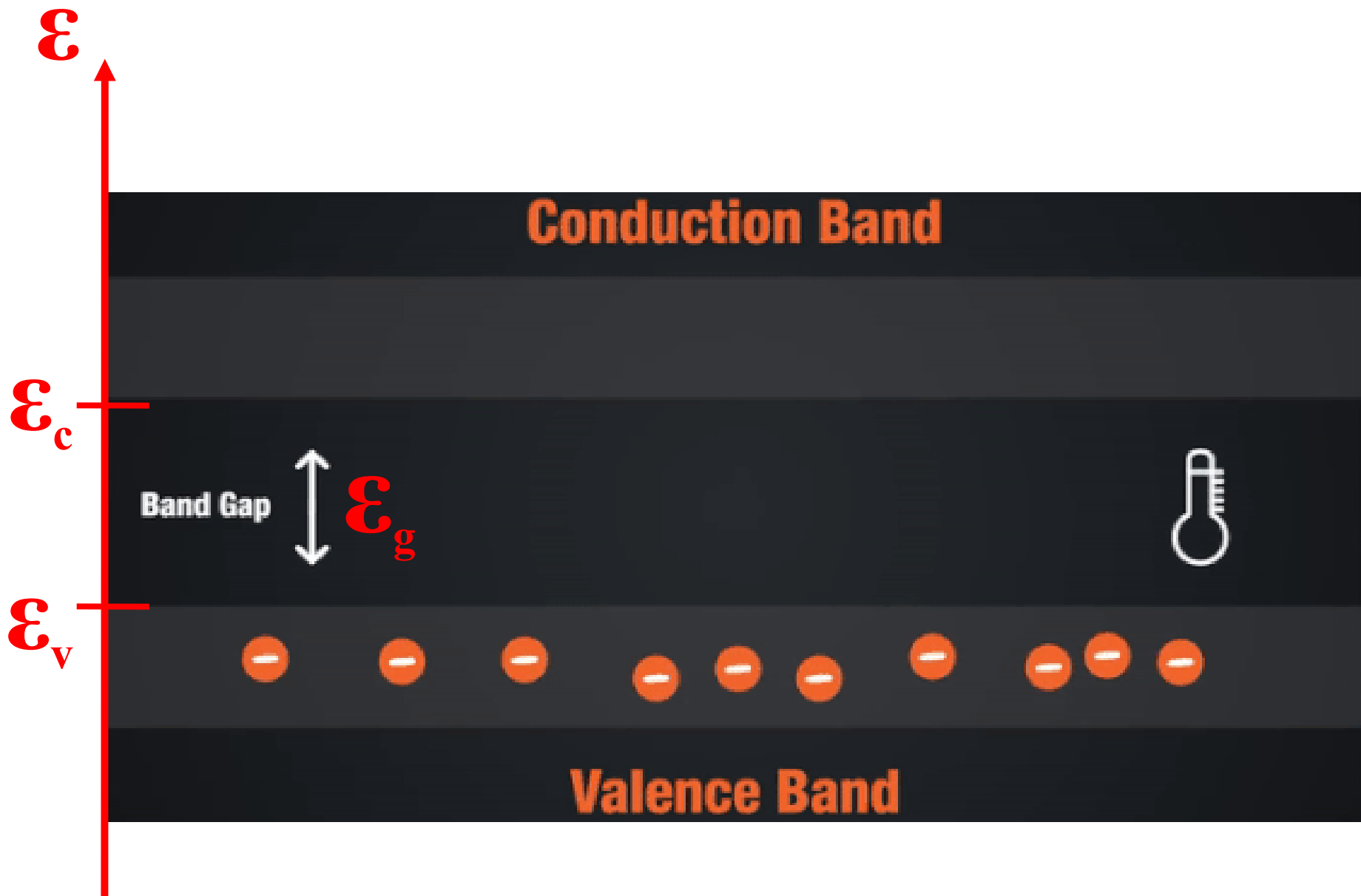
Banda de conducción



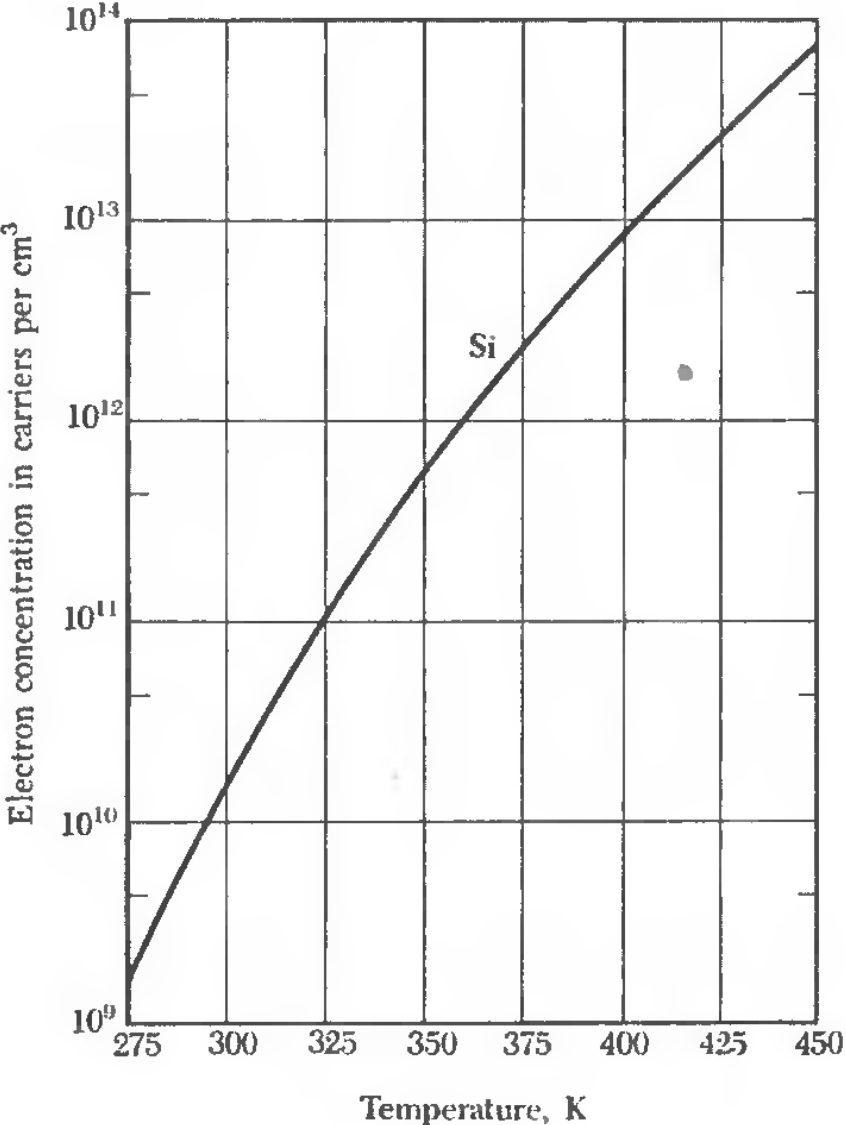
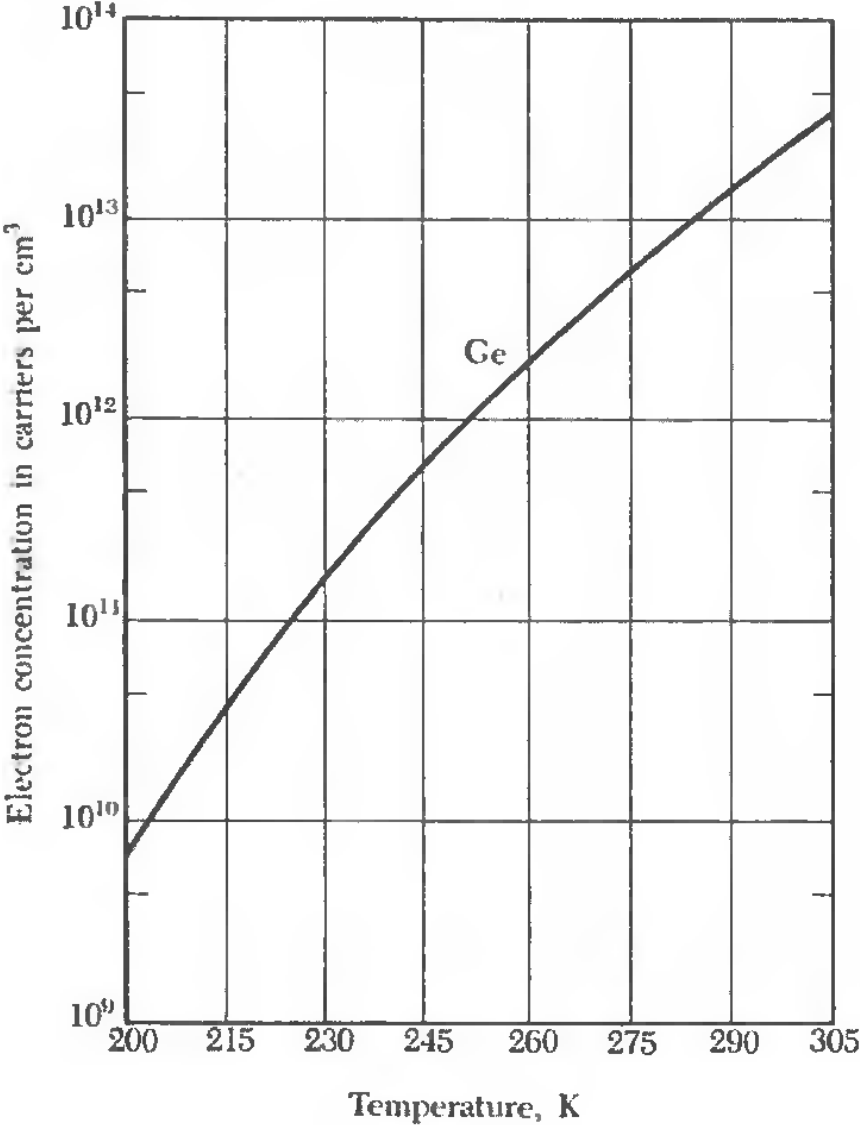
p-type intrin. *n*-type

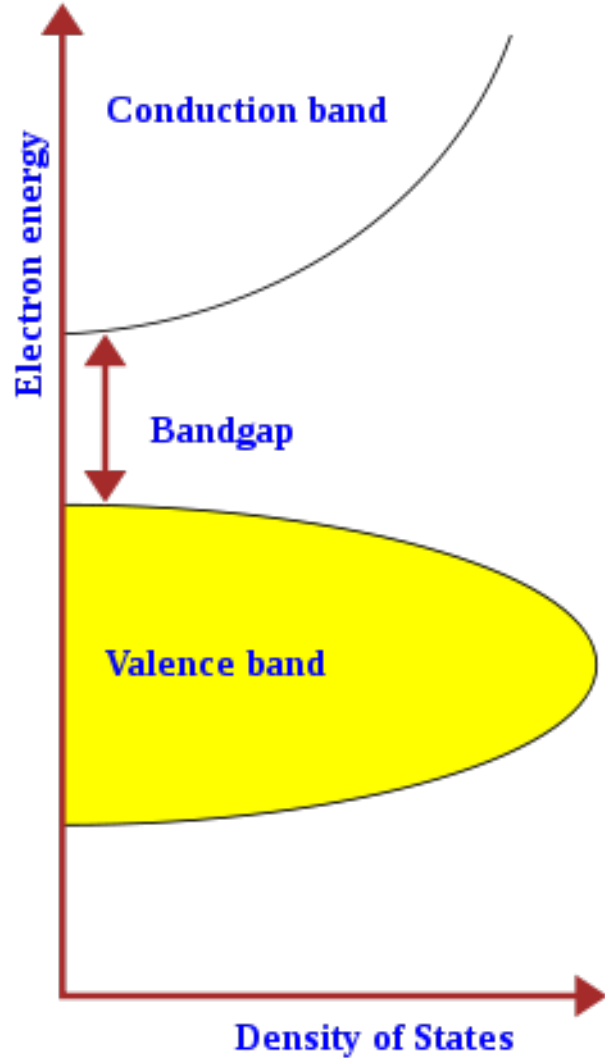
Metal Semimetal Semiconductor Insulator

Banda de valencia



Concentración de portadores en función de la temperatura

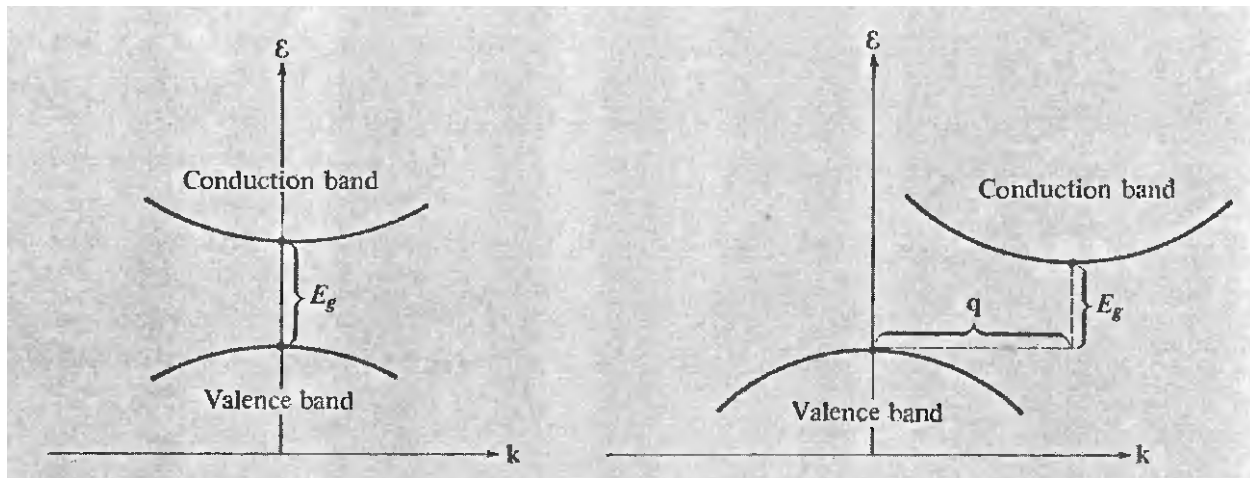




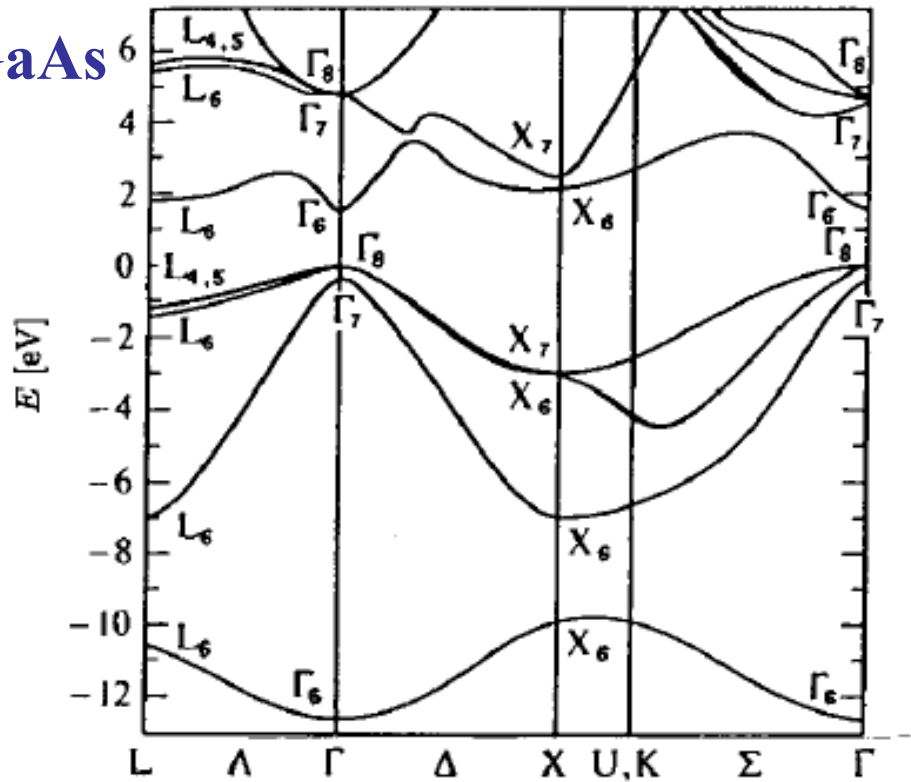
Element	$\epsilon_g(300\text{ K})$ (eV)	$\epsilon_g(T = 0)$ (eV)
C	5.48	5.4
Si	1.110	1.170
Ge	0.664	0.744

III-V compound	ϵ_g (eV)	II-VI compound	ϵ_g (eV)	I-VII compound	ϵ_g (eV)
AlSb	1.63	ZnO	3.20	AgF	2.8
GaP	2.27	ZnS	3.56	AgCl	3.25
GaAs	1.43	ZnSe	2.67	AgBr	2.68
GaSb	0.71	CdS	2.50	AgI	3.02
InP	1.26	CdSe	1.75	CuCl	3.39
InAs	0.36	CdTe	1.43	CuBr	3.07
InSb	0.18	HgS	2.27	CuI	3.11

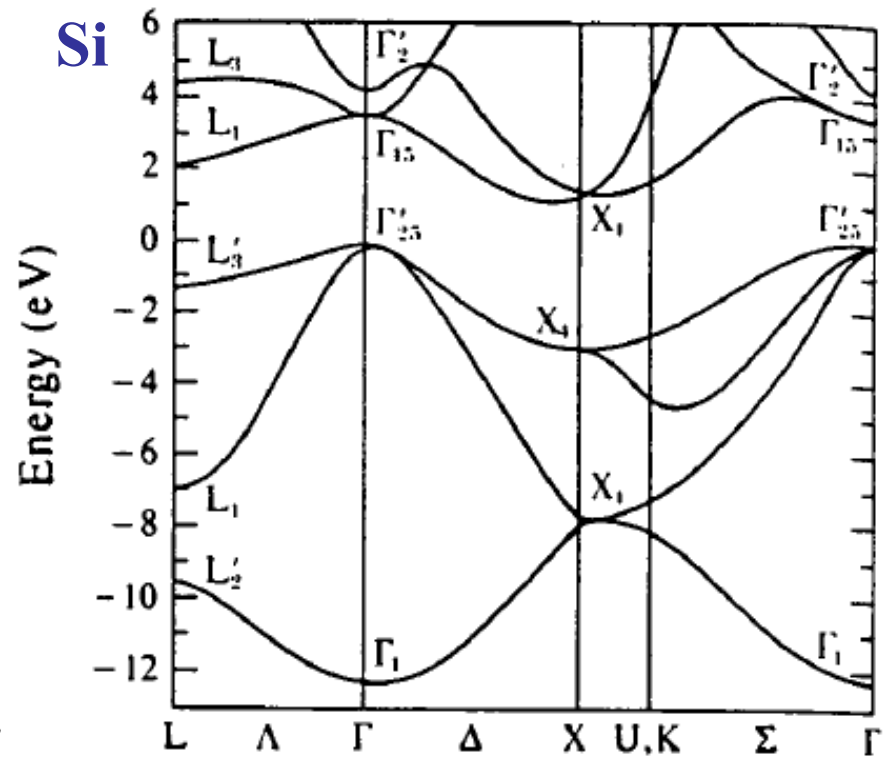
Compound	ϵ_g (eV)	Compound	ϵ_g (eV)	Compound	ϵ_g (eV)
LiF	13.7	LiCl	9.4	LiBr	7.6
NaF	11.5	NaCl	8.7	NaBr	7.5
KF	10.8	KCl	8.4	KBr	7.4
RbF	10.3	RbCl	8.2	RbBr	7.4
CsF	9.9	CsCl	8.3	CsBr	7.3



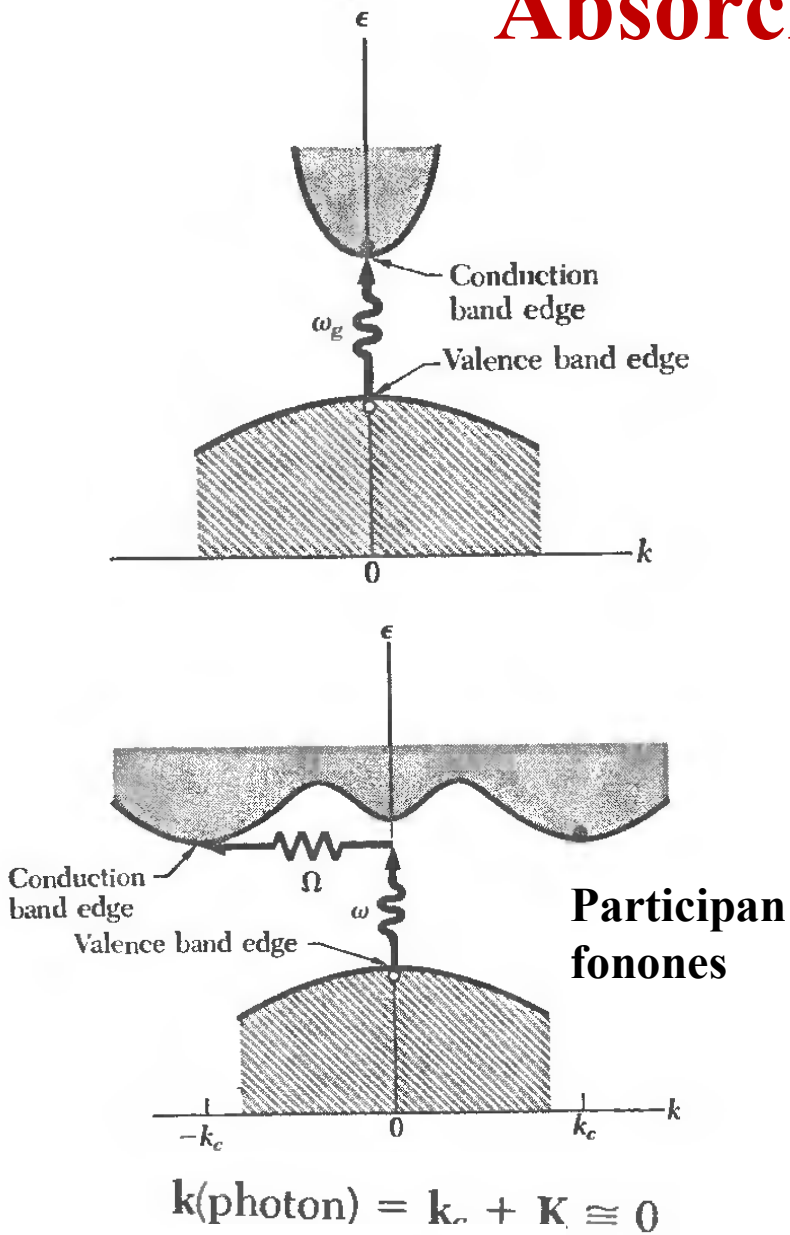
GaAs



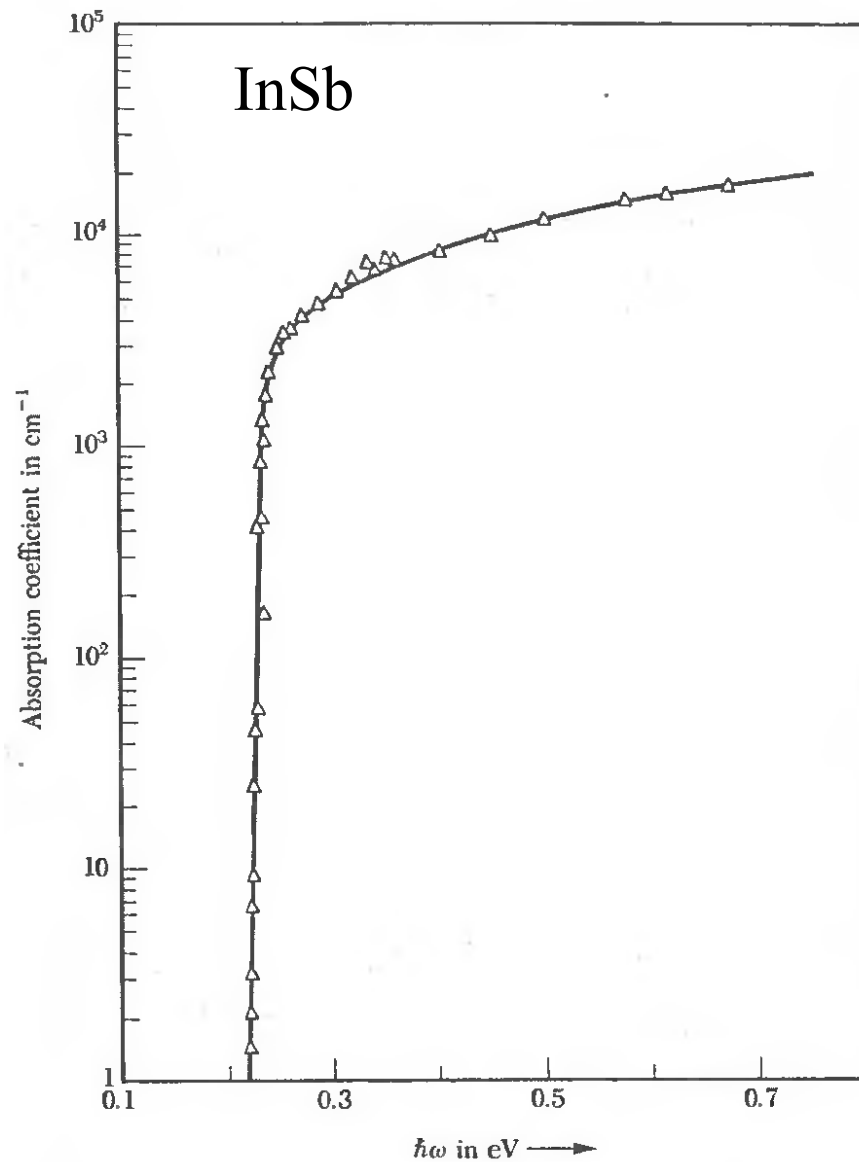
Si



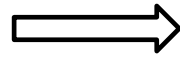
Absorción UV-Visible



$$\hbar\omega \cong E_g + \hbar\Omega$$



**Modelo
Semiclásico**



$$\dot{\mathbf{r}} = \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}},$$

$$\hbar \dot{\mathbf{k}} = -e \left[\mathbf{E}(\mathbf{r}, t) + \frac{1}{c} \mathbf{v}_n(\mathbf{k}) \times \mathbf{H}(\mathbf{r}, t) \right].$$

$$\dot{v}_k = \frac{\partial}{\partial k} \left(\frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k} \right) \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_k}{\partial k^2} \hbar \dot{k}.$$

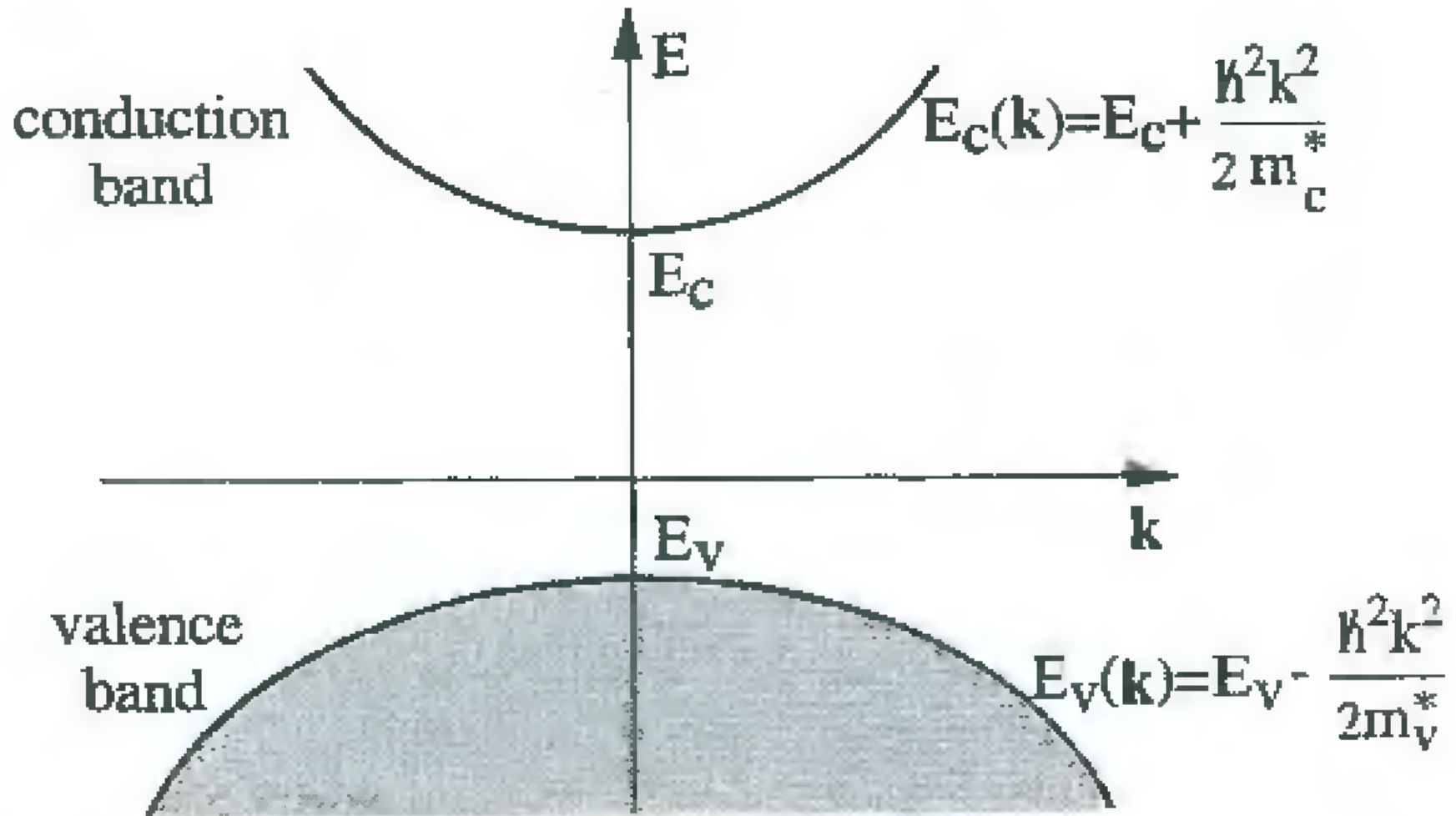
$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_k}{\partial k^2},$$

$$\left(\frac{1}{m^*} \right)_{\alpha\beta} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_\alpha \partial k_\beta}$$

Tensor masa efectiva

$$E(\mathbf{k}) = E_o(\mathbf{k}) + \sum_{\alpha\beta} \frac{\hbar^2}{2} \left(\frac{1}{m^*} \right)_{\alpha\beta} k_\alpha k_\beta$$

Muy útil en semiconductores !!!!



Agujeros (Holes)

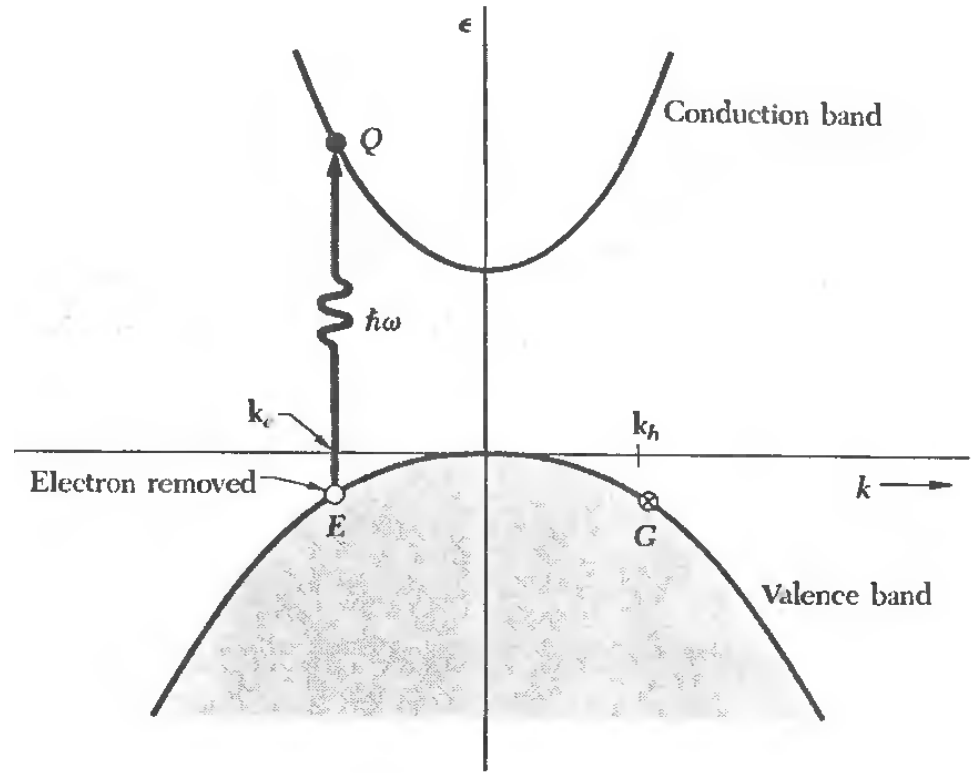
Los orbitales vacíos en una banda son denominados “holes”.
Un hole actúa bajo un campo E o B como si tuviera carga +e.

1) $\mathbf{k}_h = -\mathbf{k}_e$

En una banda llena

$$\Sigma \mathbf{k} = \mathbf{0}.$$

debido a la simetría de
inversión $\mathbf{r} \rightarrow -\mathbf{r}$

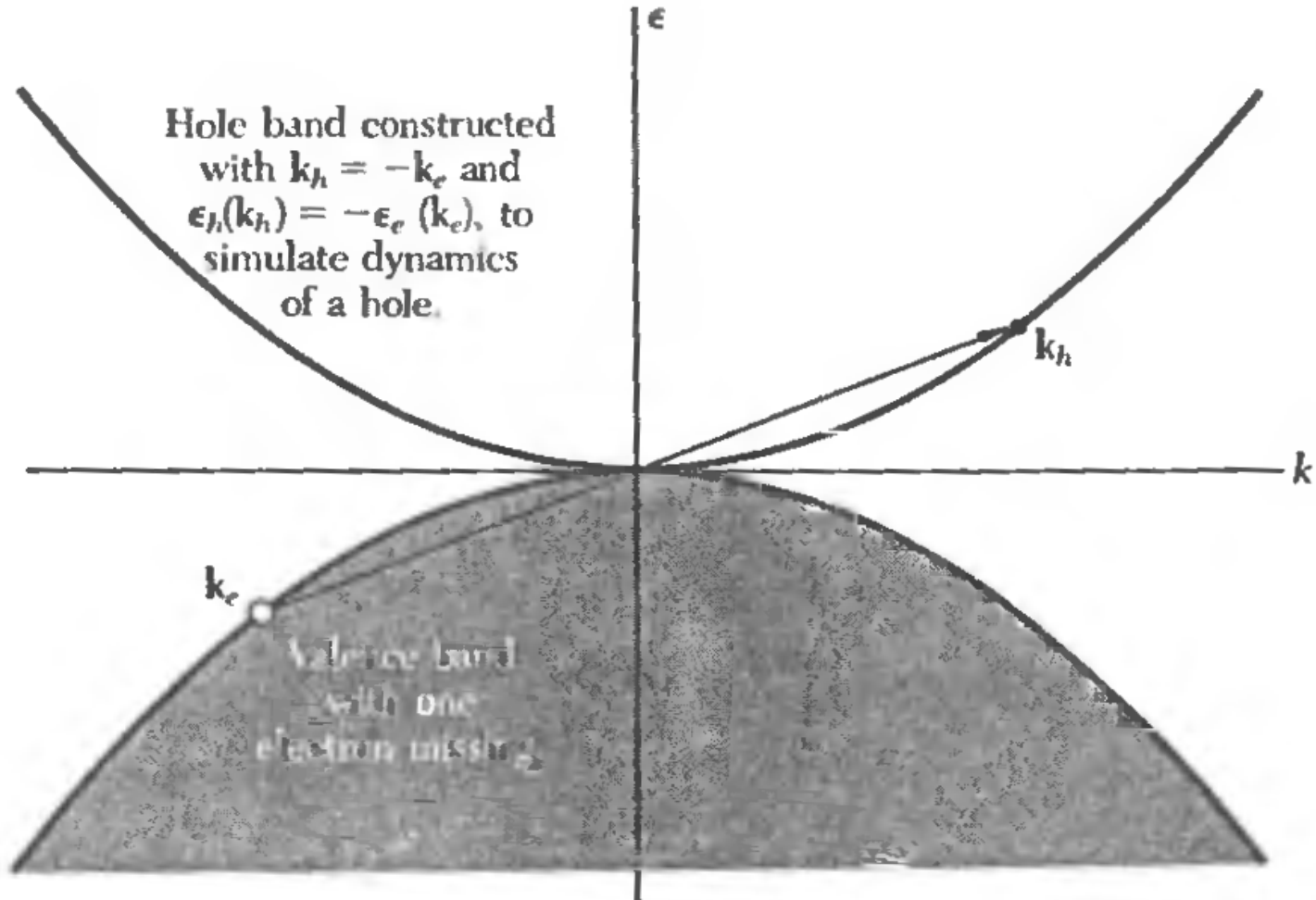
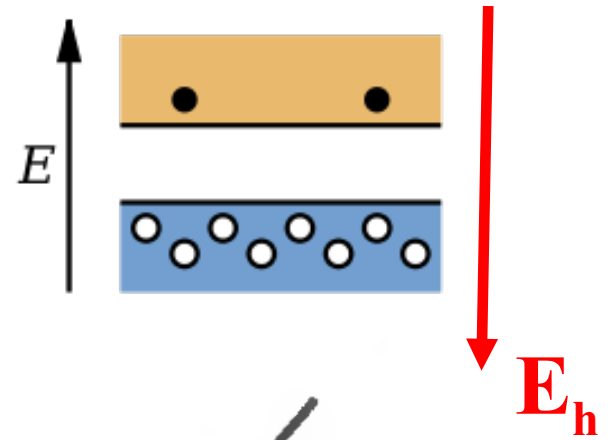


Si falta un e^- con $k=k_e$

$$\mathbf{k}_h = \sum_{k \neq k_e} \mathbf{k} = \sum_{k \neq k_e} \mathbf{k} + \mathbf{k}_e - \mathbf{k}_e = \sum \mathbf{k} - \mathbf{k}_e = -\mathbf{k}_e$$

2)

$$\epsilon_h(k_h) = -\epsilon_e(k_e)$$



3)

$$\mathbf{v}_h = \mathbf{v}_e$$

La velocidad del hole es igual a la velocidad del electrón faltante.

Se ve claramente en la Figura anterior que $\nabla \epsilon_h(\mathbf{k}_h) = \nabla \epsilon_e(\mathbf{k}_e)$

4)

$$m_h = -m_e$$

5)

$$\hbar \frac{d\mathbf{k}_h}{dt} = e(\mathbf{E} + \frac{1}{c} \mathbf{v}_h \times \mathbf{B})$$

$$\hbar \frac{d\mathbf{k}_e}{dt} = -e(\mathbf{E} + \frac{1}{c} \mathbf{v}_e \times \mathbf{B})$$

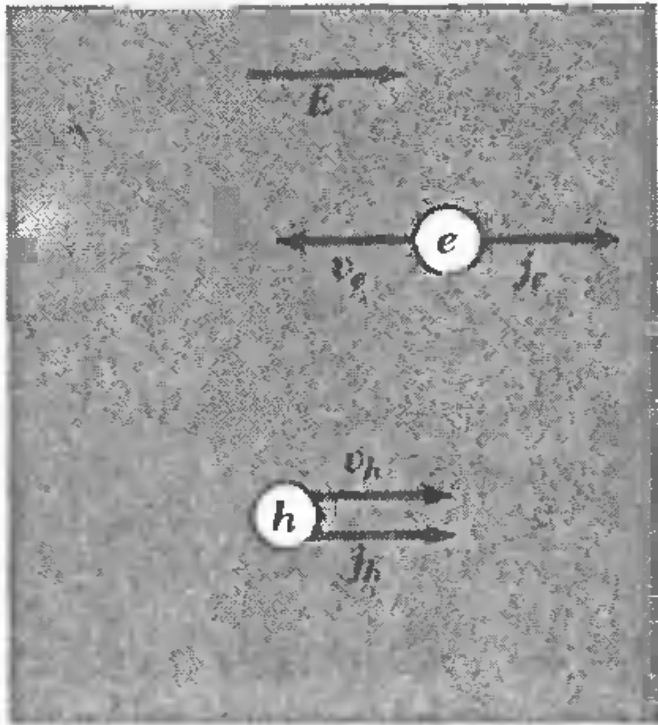
Remplazando:

$$\mathbf{k}_e \rightarrow -\mathbf{k}_h$$

$$\mathbf{v}_e \rightarrow \mathbf{v}_h$$

$$6) \quad \mathbf{j} = (-e) \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}), = (+e) \int_{\text{unoccupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}).$$

$$0 = \int_{\text{zone}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) = \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}) + \int_{\text{unoccupied}} \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}(\mathbf{k}),$$



Si en un SC hay **electrones** en la banda de conducción y **holes** en la banda de valencia:

Los dos tipos de portadores contribuyen a la corriente.

conductividad \rightarrow electrons + holes

$$\sigma = (ne\mu_e + pe\mu_h)$$

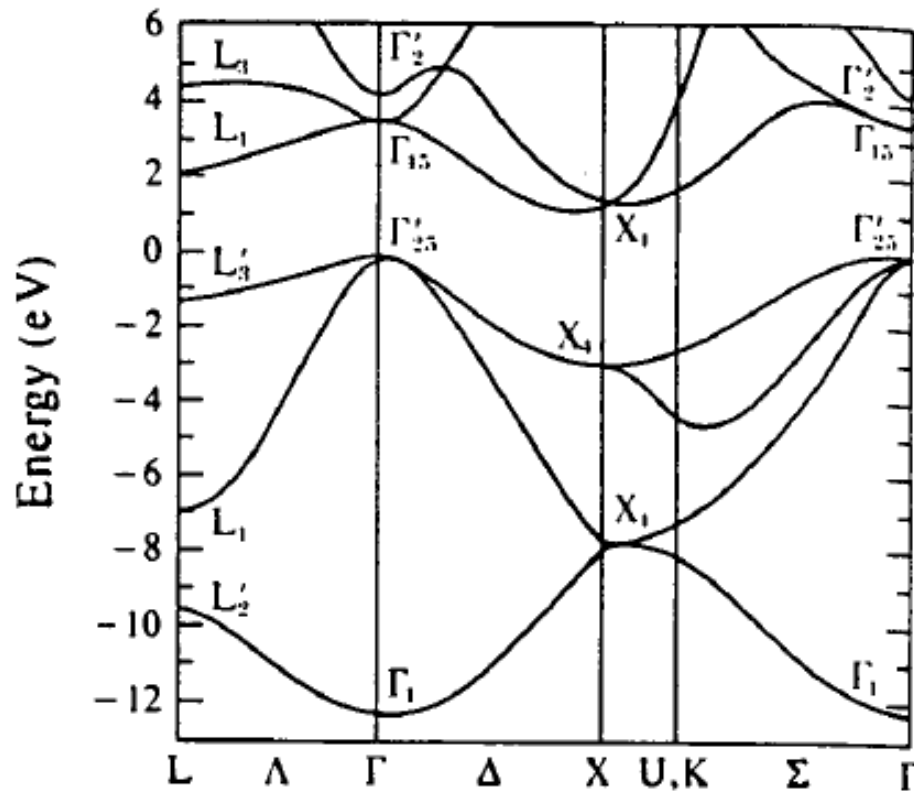
$$\mu_e = e\tau_e/m_e ; \quad \mu_h = e\tau_h/m_h$$

Table 3 Carrier mobilities at room temperature, in $\text{cm}^2/\text{V}\cdot\text{s}$

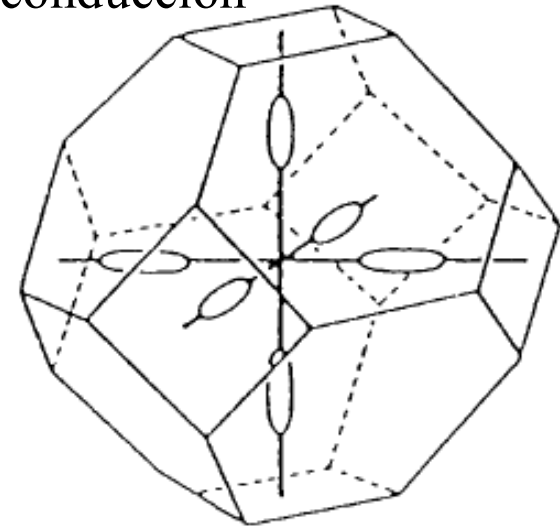
Crystal	Electrons	Holes	Crystal	Electrons	Holes
Diamond	1800	1200	GaAs	8000	300
Si	1350	480	GaSb	5000	1000
Ce	3600	1800	PbS	550	600
InSb	800	450	PbSe	1020	930
InAs	30000	450	PbTe	2500	1000
InP	4500	100	AgCl	50	—
AlAs	280	—	KBr (100 K)	100	—
AlSb	900	400	SiC	100	10–20

Algunos ejemplos del tensor masa efectiva de e^- y h^+ en semiconductores

Si



Superficie de energía cte (baja) para la banda de conducción

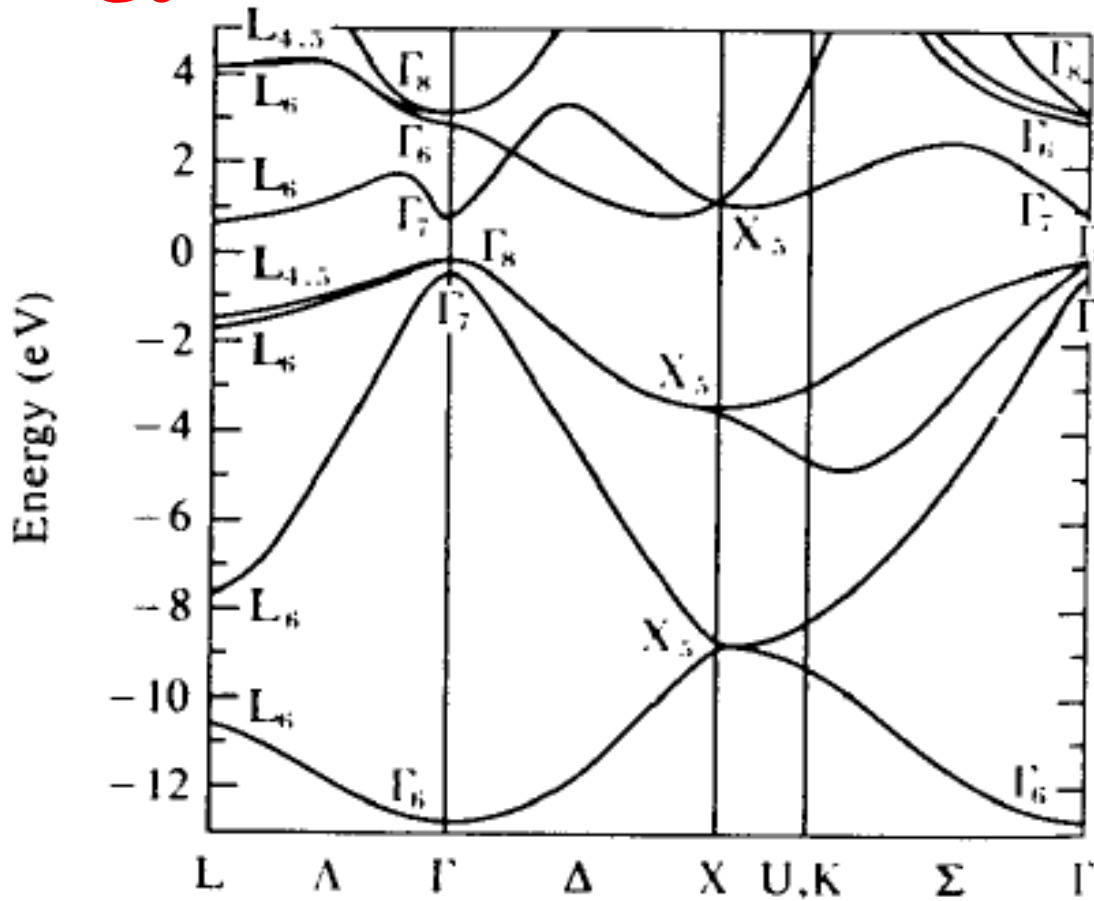


$$k_c = (2\pi/a)(0, 0, \pm 0.85)$$

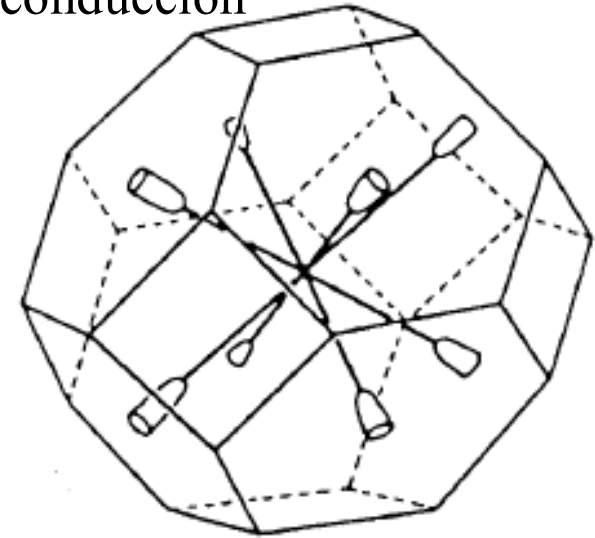
$$\epsilon_{\mathbf{k}} = \hbar^2 \left[\frac{k_x^2 + k_y^2}{2m_{n\perp}^*} + \frac{(k_z - k_{cz})^2}{2m_{n\parallel}^*} \right]$$

$$m_{n\parallel}^* = 0.916 m_e, \quad m_{n\perp}^* = 0.191 m_e$$

Ge



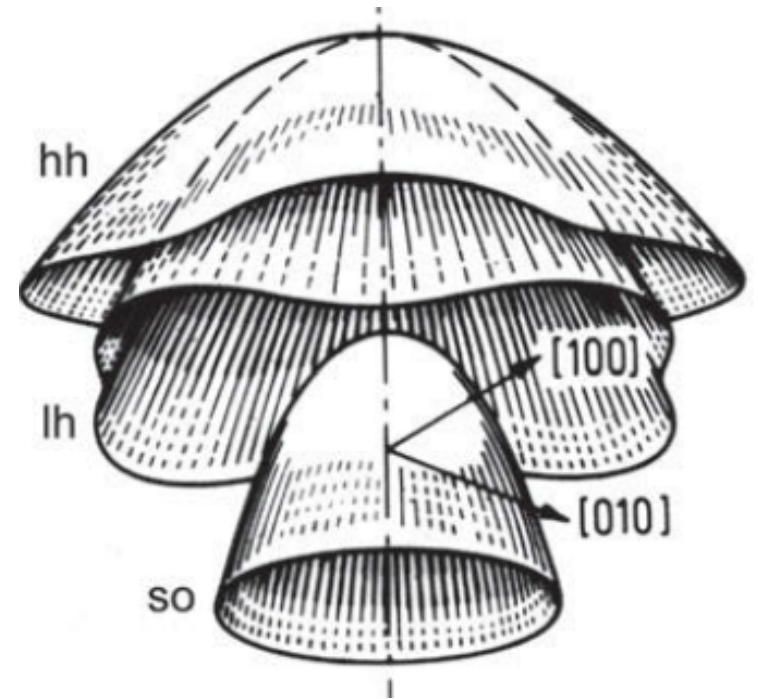
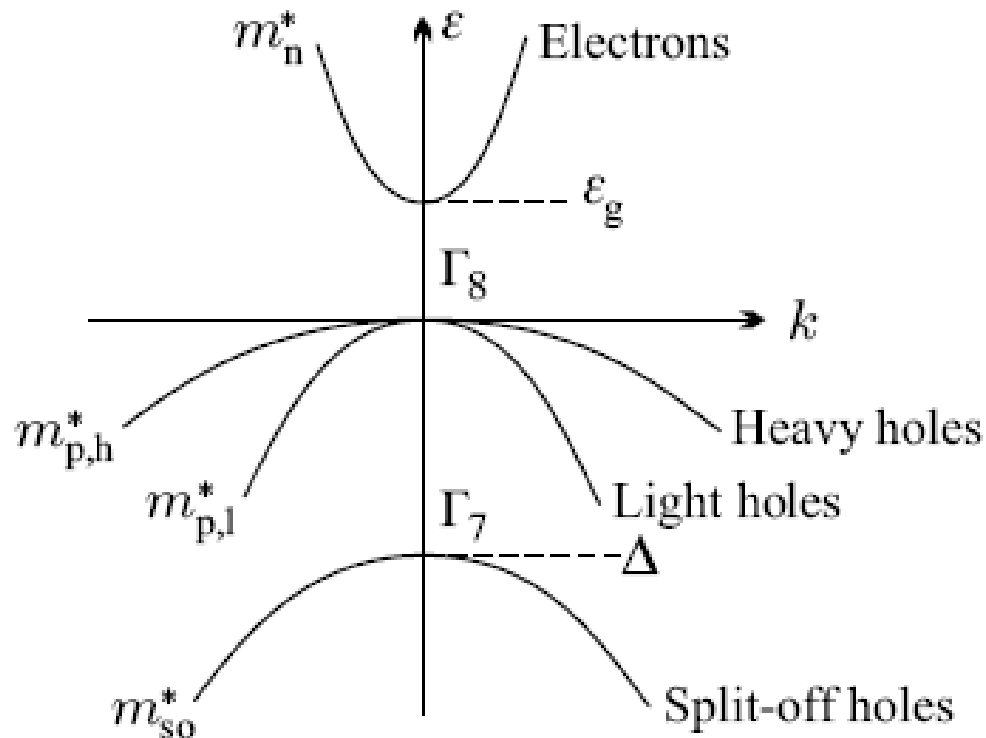
Superficie de energía cte (baja) para la banda de conducción



$$k_c = L = (2\pi/a)\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

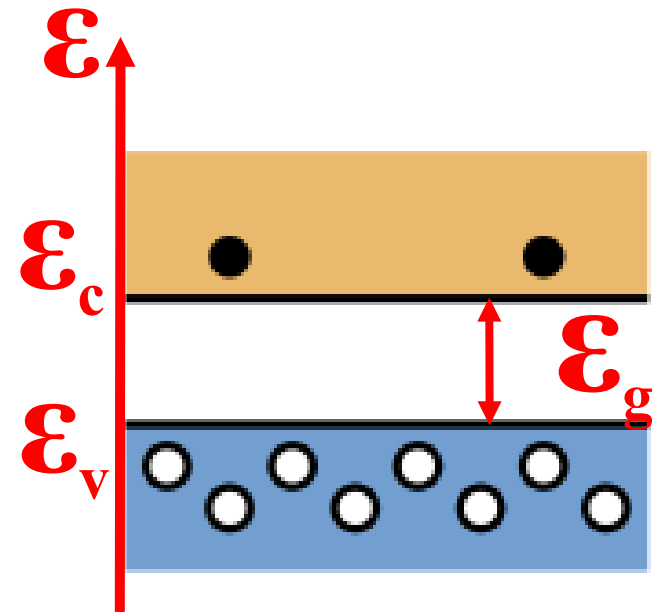
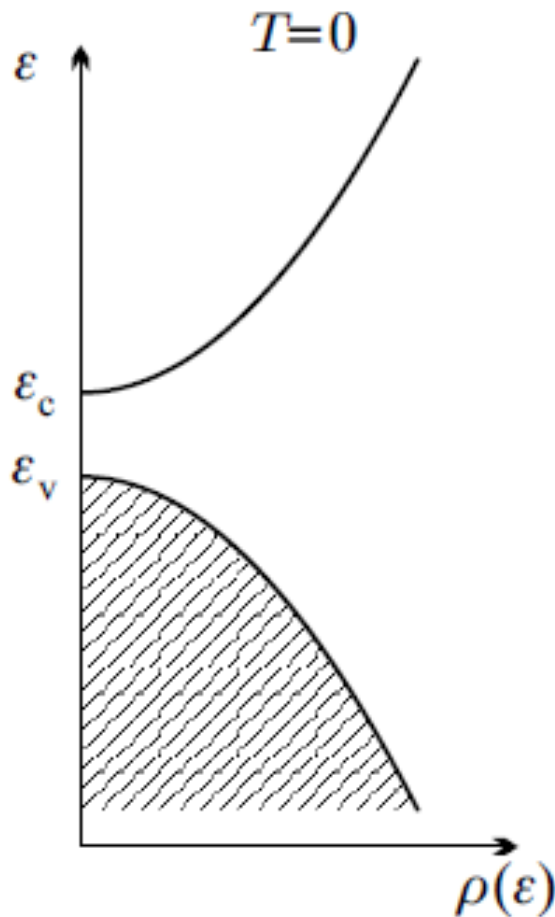
$$m_{n\parallel}^* = 1.588 m_e \quad \text{and}$$

$$m_{n\perp}^* = 0.082 m_e .$$



Crystal	m_n^*/m_e	$m_{p,h}^*/m_e$	$m_{p,l}^*/m_e$	m_{so}^*/m_e
GaAs	0.066	0.47	0.07	0.15
GaSb	0.042	0.35	0.05	0.12
InP	0.077	0.56	0.12	0.12
InAs	0.024	0.43	0.026	0.14
InSb	0.014	0.39	0.016	0.43

Concentración de portadores en equilibrio térmico



Asumiremos que las bandas están caracterizadas por masas efectivas escalares

$$\rho_c(\epsilon) = \frac{1}{2\pi^2} \left(\frac{2m_n^*}{\hbar^2} \right)^{3/2} \sqrt{\epsilon - \epsilon_c},$$

$$\rho_v(\epsilon) = \frac{1}{2\pi^2} \left(\frac{2m_p^*}{\hbar^2} \right)^{3/2} \sqrt{\epsilon_v - \epsilon}$$

Densidad de electrones en la banda de conducción:

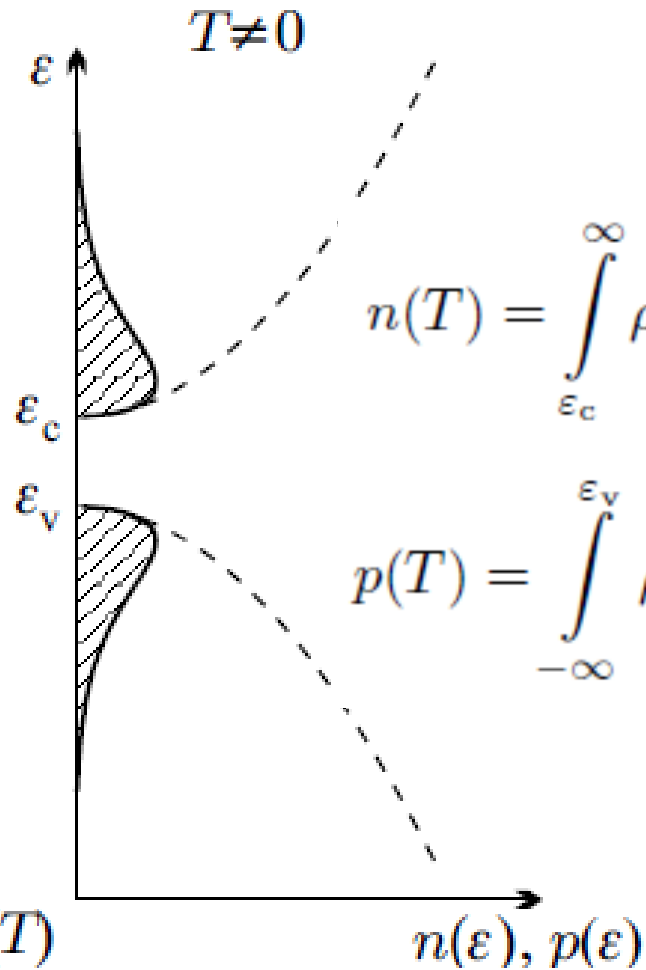
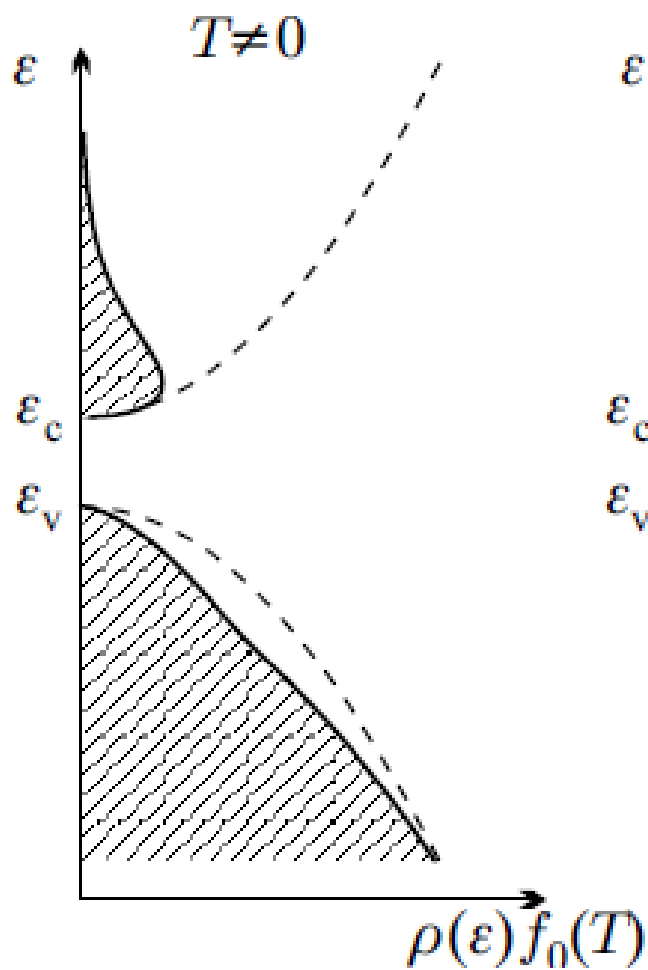
$$n(T) = \int_{\epsilon_c}^{\infty} \rho_c(\epsilon) \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} d\epsilon$$

Densidad de electrones en la banda de valencia:

$$n_v(T) = \int_{-\infty}^{\epsilon_v} \rho_v(\epsilon) \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} d\epsilon.$$

Es mas práctico trabajar con agujeros. La densidad de holes en la banda de valencia es :

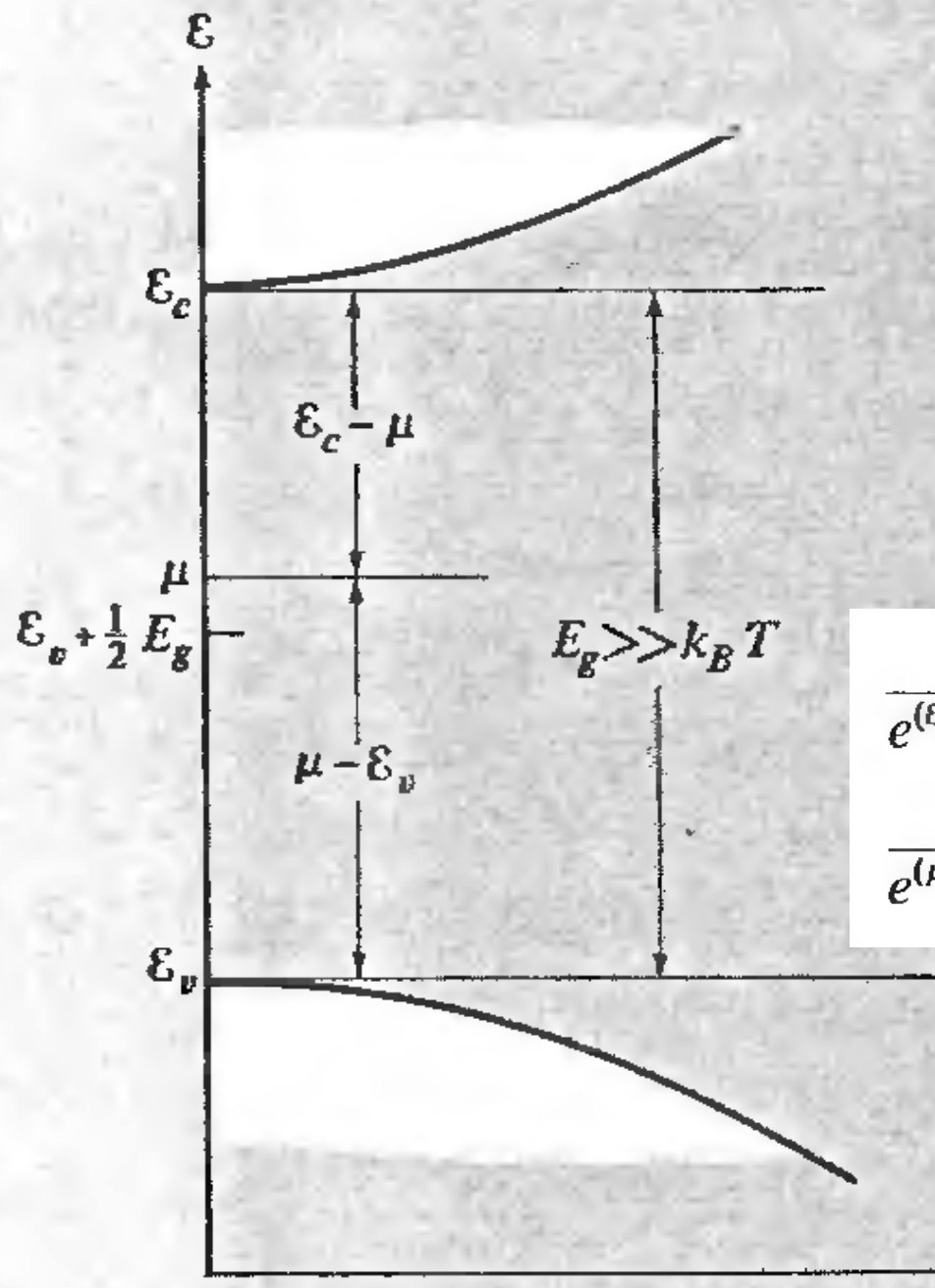
$$p(T) = \int_{-\infty}^{\epsilon_v} \rho_v(\epsilon) \left[1 - \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} \right] d\epsilon = \int_{-\infty}^{\epsilon_v} \rho_v(\epsilon) \frac{1}{e^{(\mu-\epsilon)/k_B T} + 1} d\epsilon$$



$$n(T) = \int_{\epsilon_c}^{\infty} \rho_c(\epsilon) \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} d\epsilon$$

$$p(T) = \int_{-\infty}^{\epsilon_v} \rho_v(\epsilon) \frac{1}{e^{(\mu-\epsilon)/k_B T} + 1} d\epsilon$$

$\mu?$



$$\epsilon_c - \mu \gg k_B T,$$

$$\mu - \epsilon_v \gg k_B T.$$

$$\frac{1}{e^{(\epsilon - \mu)/k_B T} + 1} \approx e^{-(\epsilon - \mu)/k_B T}, \quad \epsilon > \epsilon_c;$$

$$\frac{1}{e^{(\mu - \epsilon)/k_B T} + 1} \approx e^{-(\mu - \epsilon)/k_B T}, \quad \epsilon < \epsilon_v.$$

$$n(T) = \int_{\varepsilon_c}^{\infty} \rho_c(\varepsilon) e^{-(\varepsilon - \mu)/k_B T} d\varepsilon.$$

Sumando y restando ε_c en el exponente:

$$n(T) = N_c(T) e^{-(\varepsilon_c - \mu)/k_B T}$$

donde:

$$N_c(T) = \int_{\varepsilon_c}^{\infty} \rho_c(\varepsilon) e^{-(\varepsilon - \varepsilon_c)/k_B T} d\varepsilon$$

Usando la densidad de estados anterior, la integral da:

$$N_c(T) = 2 \left(\frac{m_n^* k_B T}{2\pi \hbar^2} \right)^{3/2}$$

De manera análoga para de densidad de holes

$$p(T) = \int_{-\infty}^{\varepsilon_v} \rho_v(\varepsilon) \frac{1}{e^{(\mu-\varepsilon)/k_B T} + 1} d\varepsilon$$

Sumando y restando ε_v en el exponente:

$$p(T) = P_v(T) e^{-(\mu-\varepsilon_v)/k_B T}$$

donde:

$$P_v(T) = \int_{-\infty}^{\varepsilon_v} \rho_v(\varepsilon) e^{-(\varepsilon_v-\varepsilon)/k_B T} d\varepsilon$$

$$P_v(T) = 2 \left(\frac{m_p^* k_B T}{2\pi \hbar^2} \right)^{3/2}$$

Por lo tanto: $n(T) = N_c(T) e^{-(\epsilon_c - \mu)/k_B T}$

$$p(T) = P_v(T) e^{-(\mu - \epsilon_v)/k_B T}$$

$$n(T) p(T) = N_c(T) P_v(T) e^{-(\epsilon_c - \epsilon_v)/k_B T}$$

Ley de acción de masas

Para un semiconductor a una dada temperatura, el producto de la concentración de electrones en la banda de conducción por la concentración de holes en la banda de valencia es constante.

Para obtener este resultado no hemos supuesto nada respecto al origen de los portadores: pueden ser intrínsecos o extrínsecos (impurezas).

Semiconductor intrínseco $\implies n(T) = p(T)$

Se la denomina **concentración de portadores intrínsecos** $n_i(T)$

$$n(T) p(T) = N_c(T) P_v(T) e^{-(\varepsilon_c - \varepsilon_v)/k_B T}$$

$$n_i(T) = \sqrt{N_c(T) P_v(T)} e^{-(\varepsilon_c - \varepsilon_v)/2k_B T}$$

$$= \sqrt{N_c(T) P_v(T)} e^{-\varepsilon_g/2k_B T}$$

$$n_i(T) = 2 \left(\frac{k_B T}{2\pi \hbar^2} \right)^{3/2} (m_n^* m_p^*)^{3/4} e^{-\varepsilon_g/2k_B T}$$

Para obtener valores numéricos es conveniente escribirla así:

$$n_i(T) = 2.5 \left(\frac{m_n^*}{m_e} \right)^{3/4} \left(\frac{m_p^*}{m_e} \right)^{3/4} \left(\frac{T}{300 \text{ K}} \right)^{3/2} e^{-\varepsilon_g/2k_B T} \times 10^{19} / \text{cm}^3$$

	E_g (eV)	n_i (cm ⁻³)
InSb	0.18	1.6×10^{16}
InAs	0.36	8.6×10^{14}
Ge	0.67	2.4×10^{13}
Si	1.124	1.0×10^{10}
GaAs	1.43	1.8×10^6
GaP	2.26	2.7×10^0
GaN	3.3	$\ll 1$

conductividad

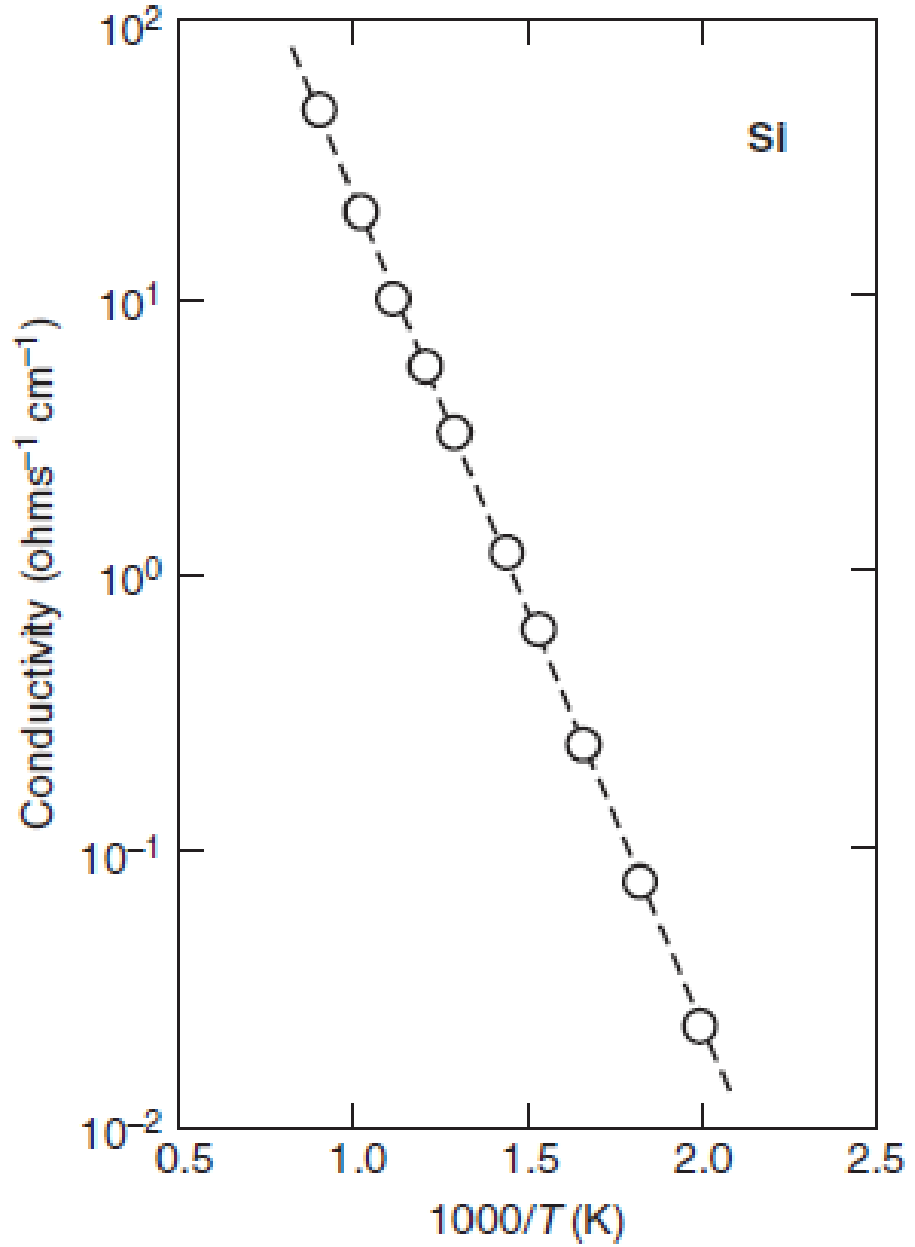
electrons + holes

$$\sigma = (ne\mu_e + pe\mu_h)$$

$$\mu_e = e\tau_e/m_e ; \quad \mu_h = e\tau_h/m_h$$

Table 3 Carrier mobilities at room temperature, in cm²/V-s

Crystal	Electrons	Holes	Crystal	Electrons	Holes
Diamond	1800	1200	GaAs	8000	300
Si	1350	480	GaSb	5000	1000
Ce	3600	1800	PbS	550	600
InSb	800	450	PbSe	1020	930
InAs	30000	450	PbTe	2500	1000
InP	4500	100	AgCl	50	—
AlAs	280	—	KBr (100 K)	100	—
AlSb	900	400	SiC	100	10–20



Intrinsic conductivity of Si plotted against inverse temperature (adapted from Moran and

M. J. (1951))

μ ?

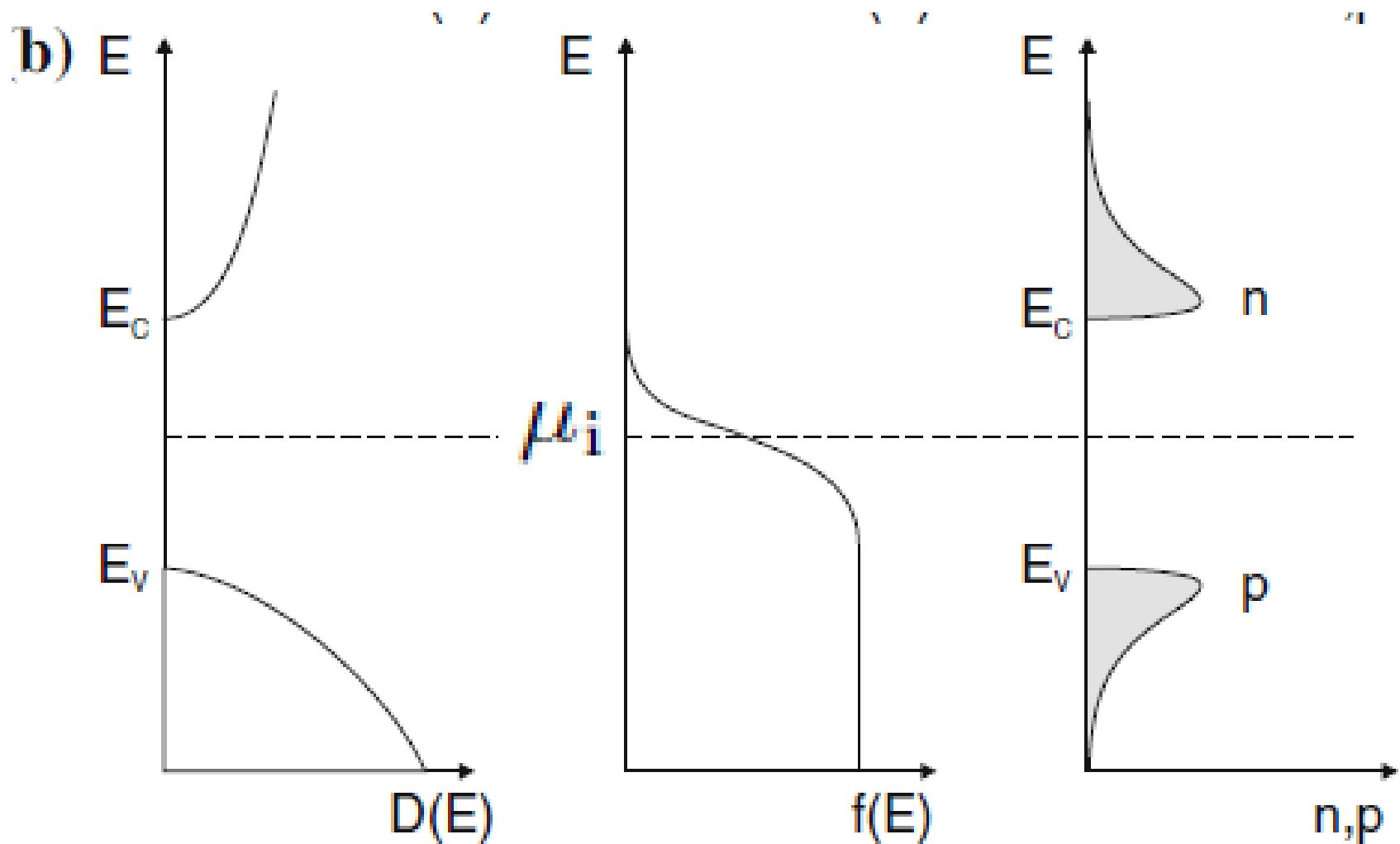
$$N_c(T)e^{-(\epsilon_c - \mu)/k_B T} = P_v(T)e^{-(\mu - \epsilon_v)/k_B T}$$

$$\frac{P_v(T)}{N_c(T)} = \exp \left[\frac{2\mu - (\epsilon_c + \epsilon_v)}{k_B T} \right]$$

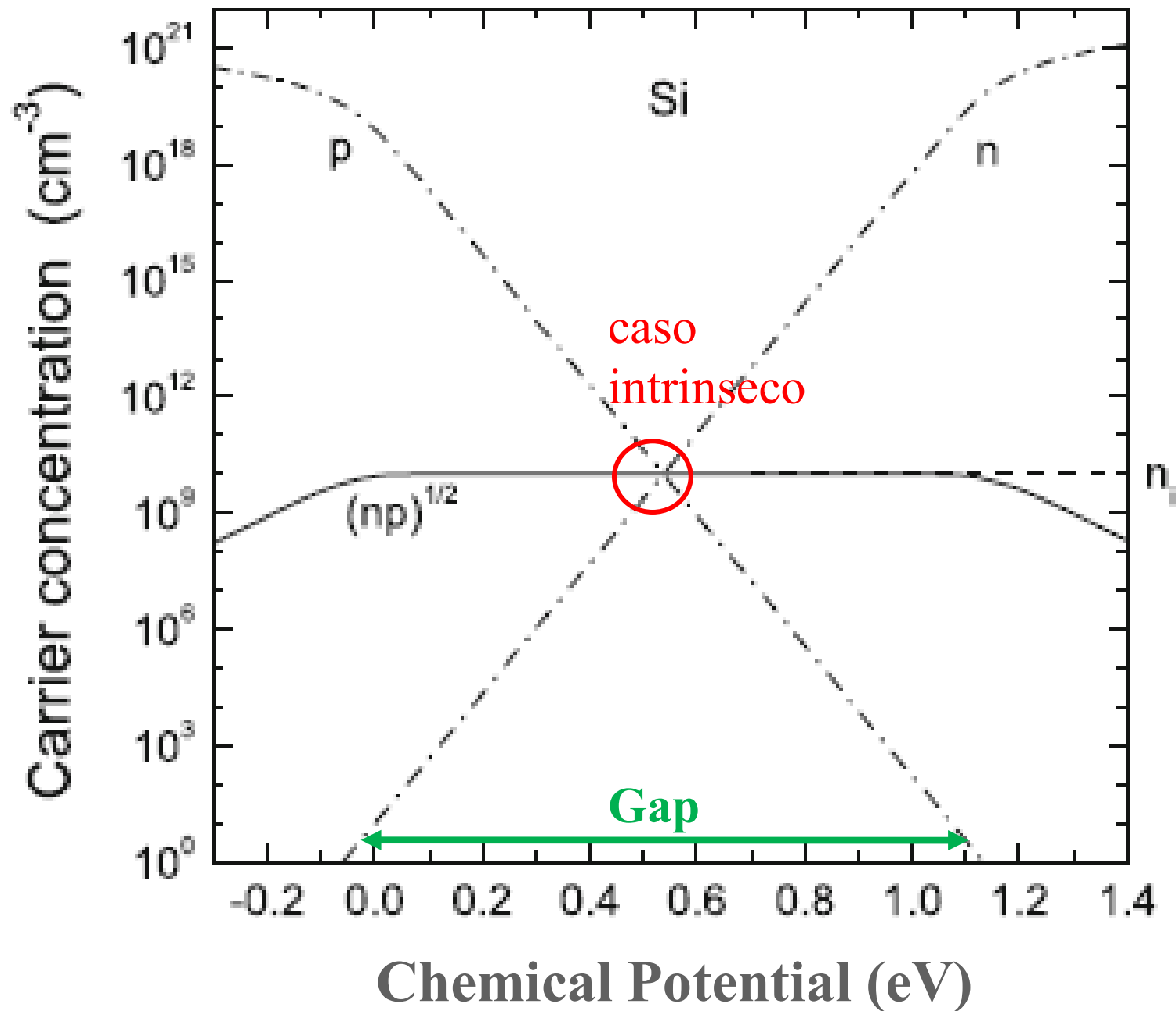
$$\mu = \frac{1}{2}(\epsilon_c + \epsilon_v) + \frac{1}{2}k_B T \ln \frac{P_v(T)}{N_c(T)}$$

$$\mu = \frac{1}{2}(\epsilon_c + \epsilon_v) + \frac{3}{4}k_B T \ln \frac{m_p^*}{m_n^*}$$

$T = 0 \implies \mu = \frac{1}{2}(\epsilon_c + \epsilon_v)$ **E_F en el medio del gap**



$$n_i = N_c(T) e^{-(\epsilon_c - \mu_i)/k_B T} = P_v(T) e^{-(\mu_i - \epsilon_v)/k_B T}$$

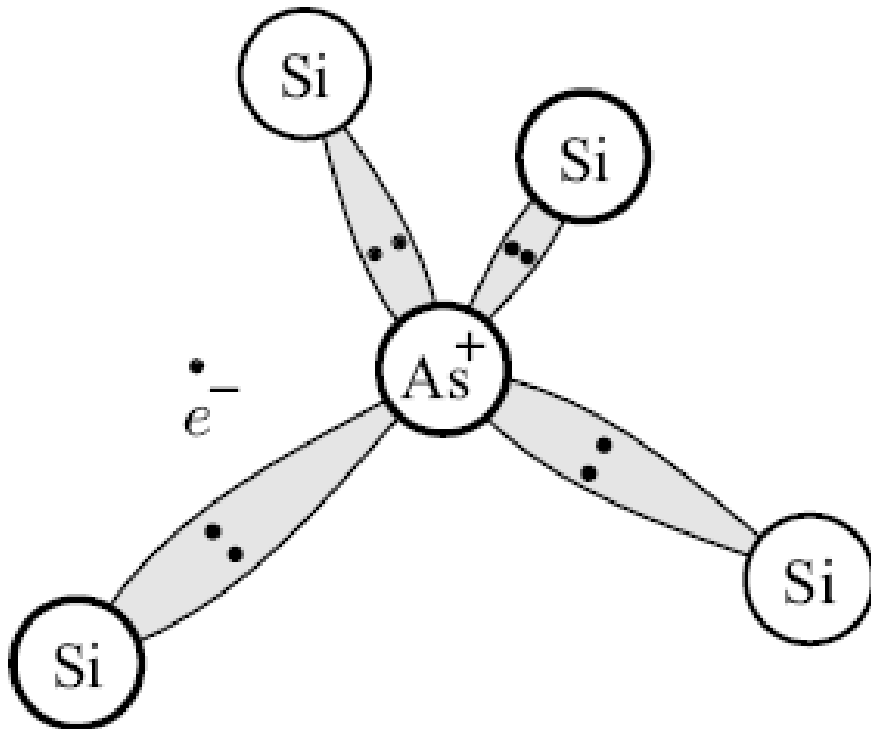


Portadores extrínsecos: impurezas

Donoras

valencia 5

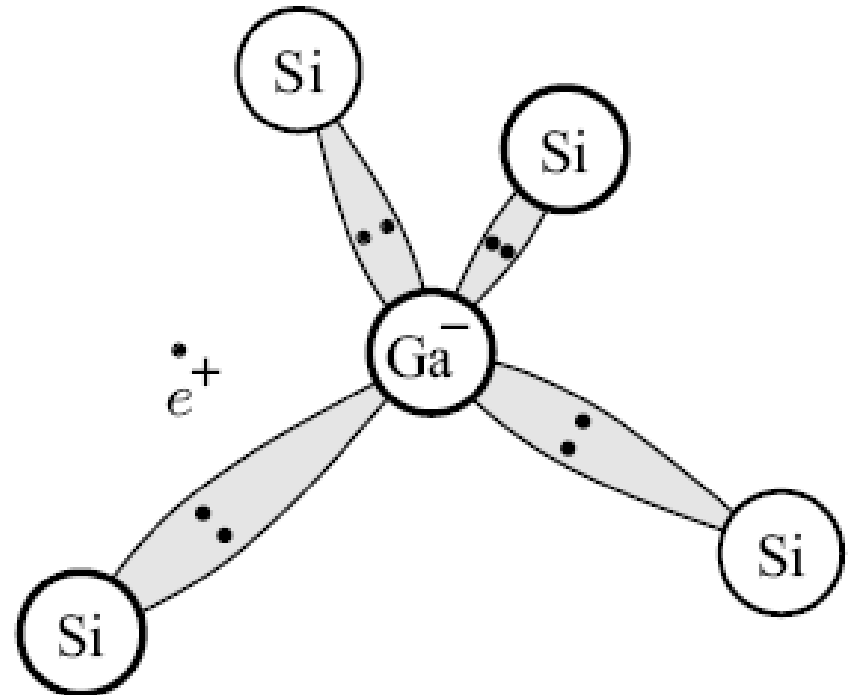
(P,As,Sb)



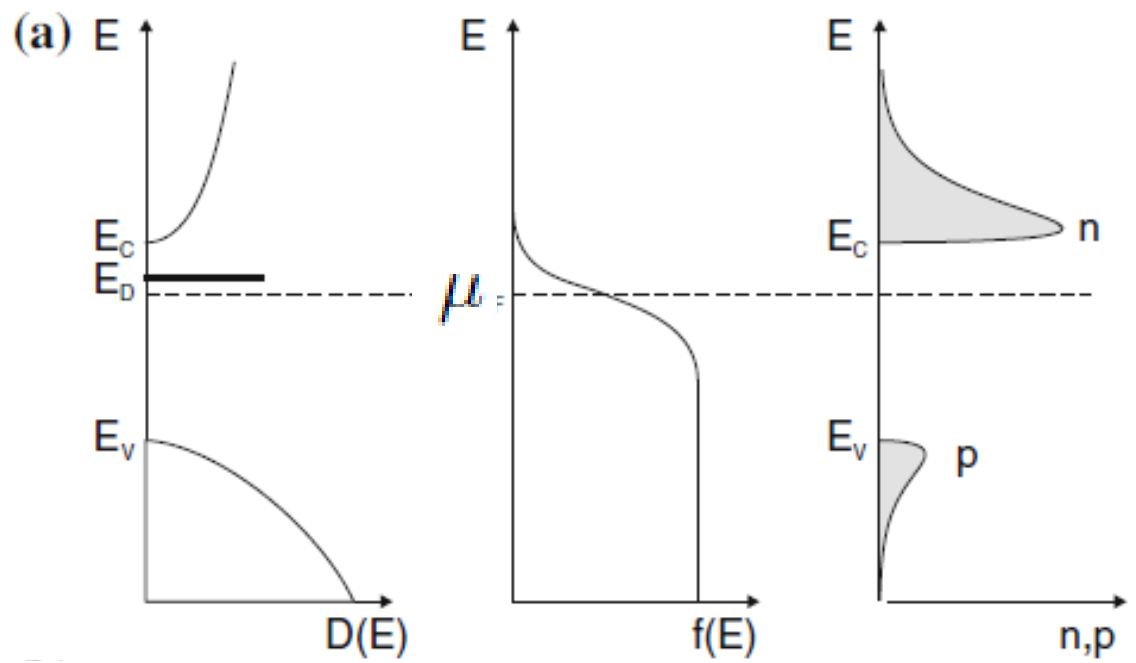
Aceptoras

valencia 3

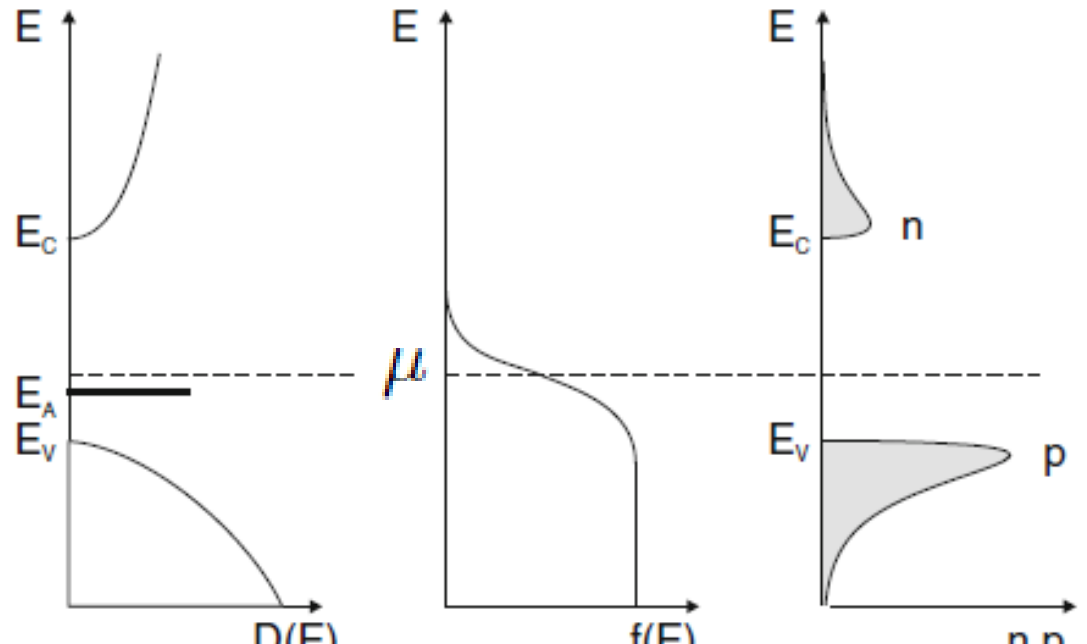
(B,Al,Ga)



Donoras



Aceptoras



Modelizaremos esta situación como si fuera un átomo de hidrogeno: un electrón en un potencial colombiano pero apantallado por el material dieléctrico

$$\begin{array}{l} \tilde{e} \rightarrow \frac{\tilde{e}}{\sqrt{\epsilon_r}} \\ m_e \rightarrow m^* \end{array} \longrightarrow \left\{ -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{\tilde{e}^2}{\epsilon_r r} \right\} \psi(r) = \epsilon \psi(r)$$

Radio de la orbita



$$r_0 = \frac{\hbar^2}{m^* (\tilde{e}^2 / \epsilon_r)} = \frac{m_e}{m^*} \epsilon_r a_0$$

a_0 , radio de Bohr del átomo de H (0.5291 Å)

Estimaciones



$$r_0^{\text{Si}} \approx 30 \text{ \AA} \quad r_0^{\text{Ge}} \approx 80 \text{ \AA}$$

Energía de ionización del átomo de H

$$\epsilon_0 = m_e \tilde{e}^4 / 2\hbar^2 = 13.6 \text{ eV}$$

Para la impureza

$$\epsilon_b = \frac{m^* (\tilde{e}^2 / \epsilon_r)^2}{2\hbar^2} = \frac{m^*}{m_e} \frac{1}{\epsilon_r^2} \frac{m_e \tilde{e}^4}{2\hbar^2}$$

$$\epsilon_b = \frac{m^*}{m_e} \frac{1}{\epsilon_r^2} \times 13.6 \text{ eV}$$

Estimaciones



20 meV for silicon

5.5 meV for germanium

Table 2 Effective masses of electrons and holes in direct gap semiconductors

Crystal	Electron m_e/m	Heavy hole m_{hh}/m	Light hole m_{lh}/m	Split-off hole m_{soh}/m	Spin-orbit Δ , eV
InSb	0.015	0.39	0.021	(0.11)	0.82
InAs	0.026	0.41	0.025	0.08	0.43
InP	0.073	0.4	(0.078)	(0.15)	0.11
GaSb	0.047	0.3	0.06	(0.14)	0.80
GaAs	0.066	0.5	0.082	0.17	0.34
Cu ₂ O	0.99	—	0.58	0.69	0.13

Table 4 Static relative dielectric constant of semiconductors

Crystal	ϵ	Crystal	ϵ
Diamond	5.5	GaSb	15.69
Si	11.7	GaAs	13.13
Ge	15.8	AlAs	10.1
InSb	17.88	AlSb	10.3
InAs	14.55	SiC	10.2
InP	12.37	Cu ₂ O	7.1

Table 5 Donor ionization energies E_d of pentavalent impurities in germanium and silicon, in meV

	P	As	Sb
Si	45.	49.	39.
Ge	12.0	12.7	9.6

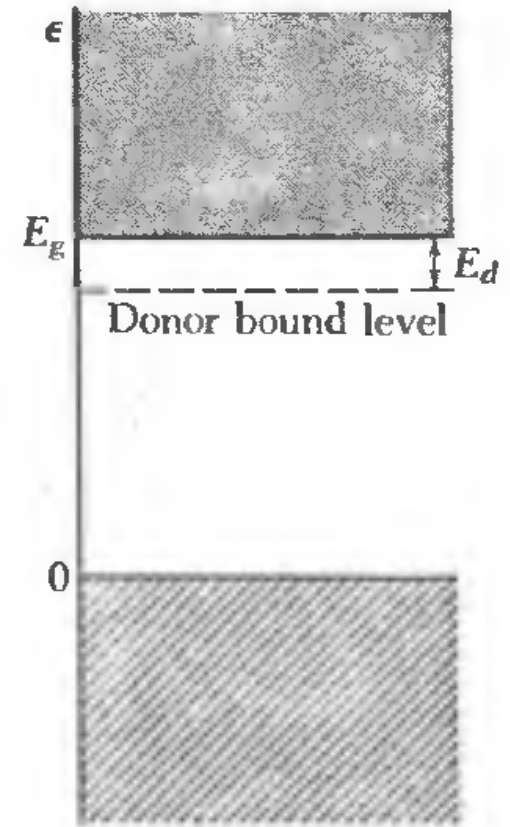
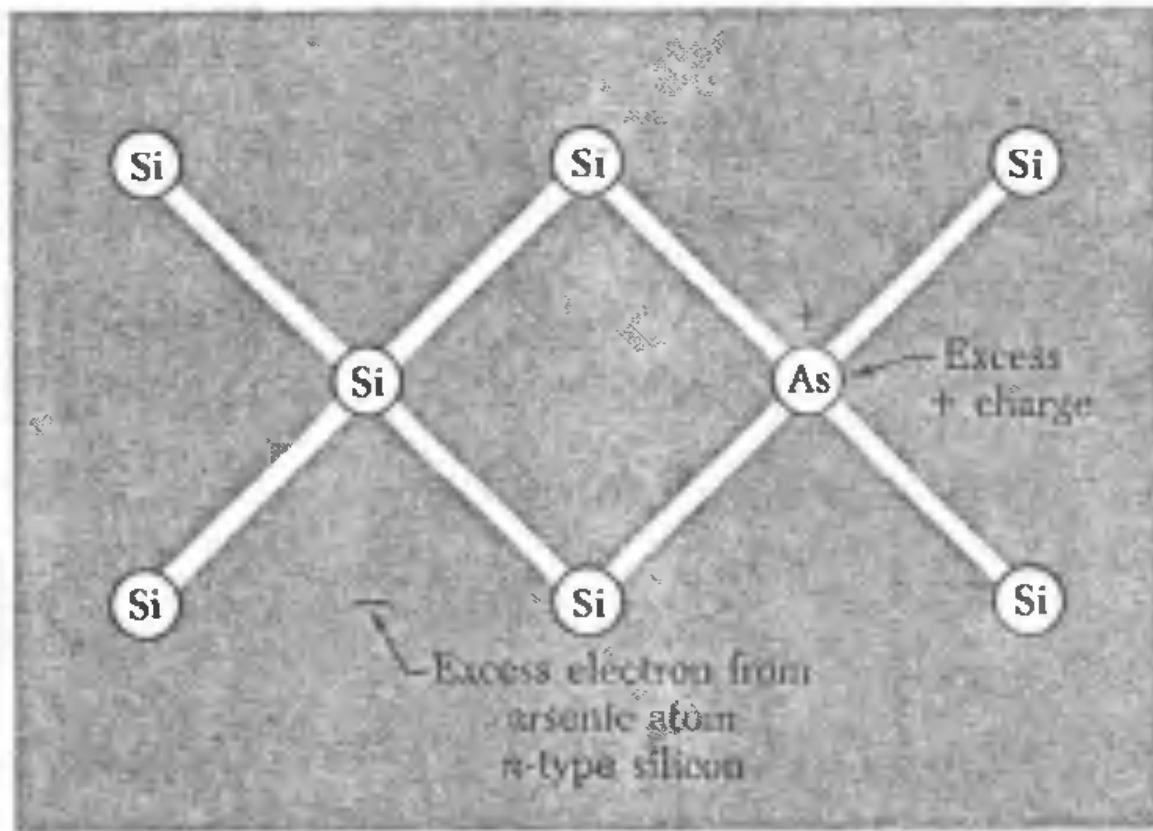
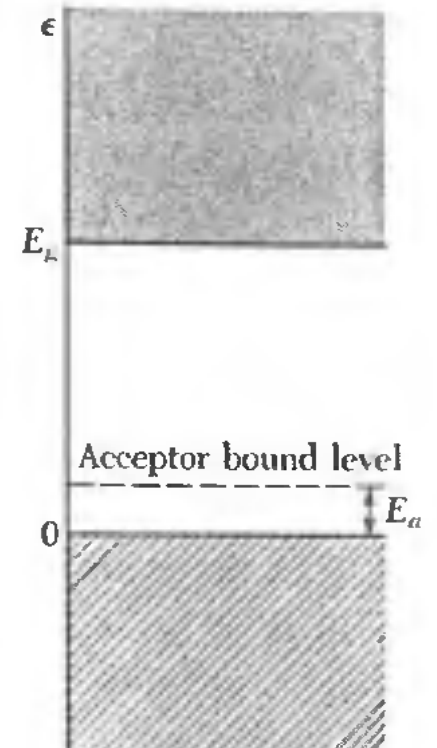
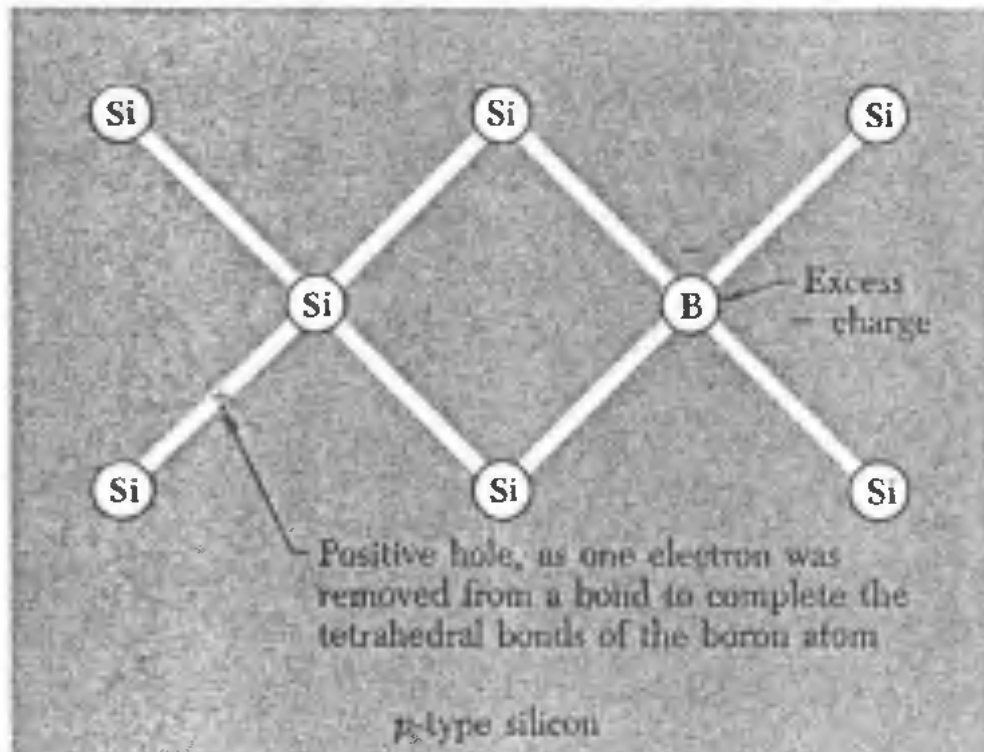
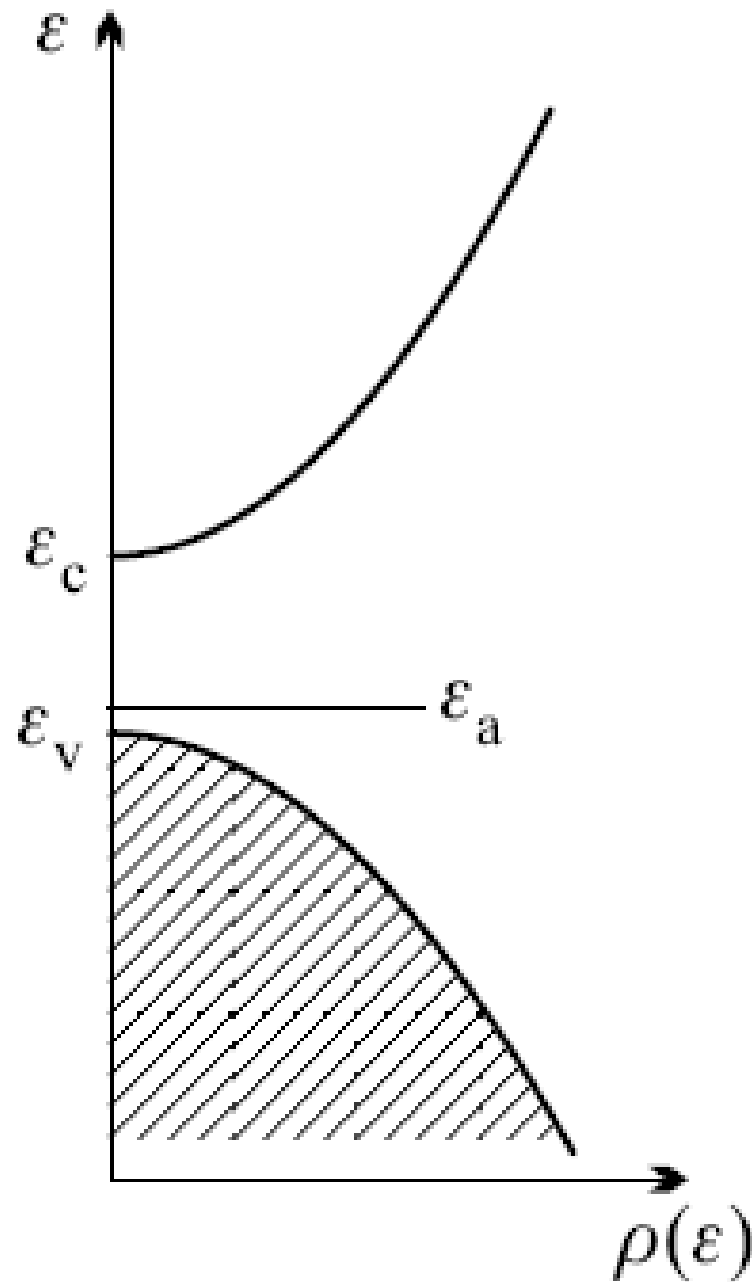
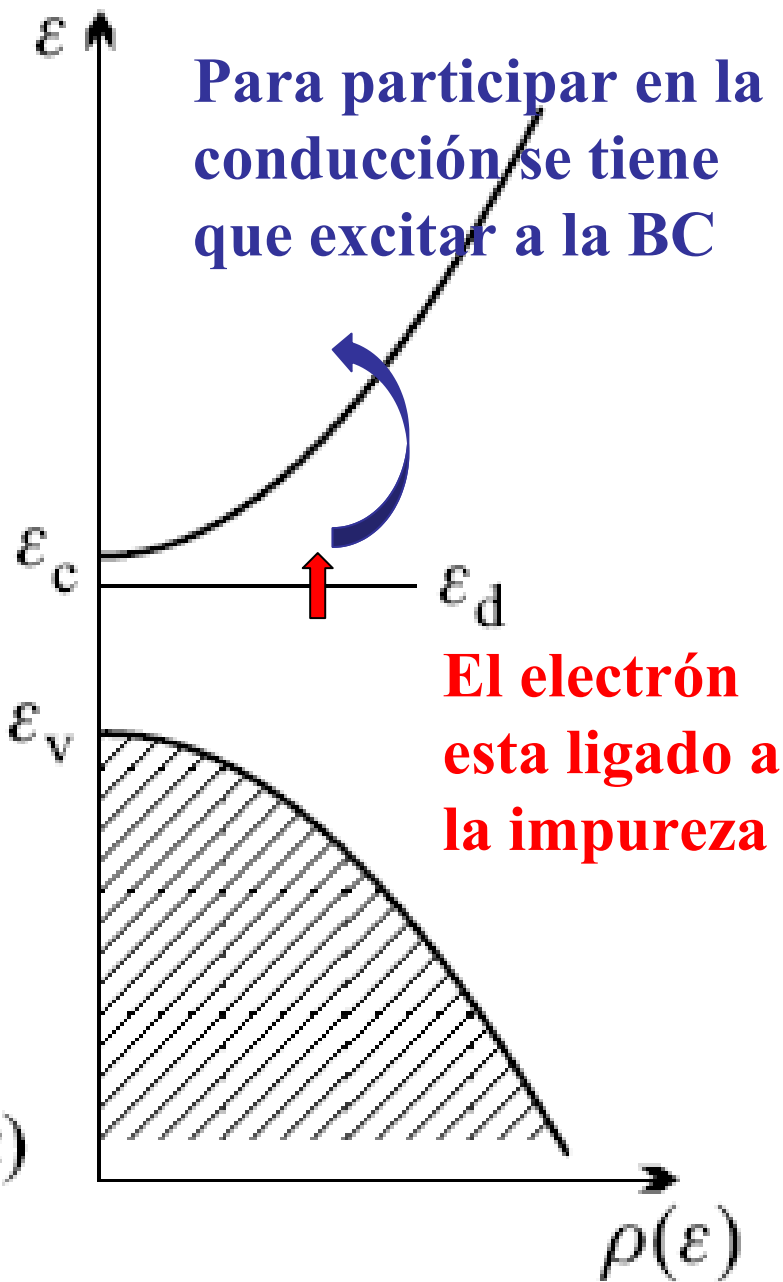


Table 6 Acceptor ionization energies E_a of trivalent impurities in germanium and silicon, in meV

	B	Al	Ga	In
Si	45.	57.	65.	157.
Ge	10.4	10.2	10.8	11.2



Para participar en la
conducción se tiene
que excitar a la BC



Densidad de portadores en semiconductores dopados

Densidad de impurezas donaras N_D $\begin{cases} N_D^0 & \text{neutras} \\ N_D^+ & \text{ionizadas} \end{cases}$

Densidad de impurezasceptoras N_A $\begin{cases} N_A^0 & \text{neutras} \\ N_A^- & \text{ionizadas} \end{cases}$

$$N_D = N_D^0 + N_D^+$$

$$N_A = N_A^0 + N_A^-$$

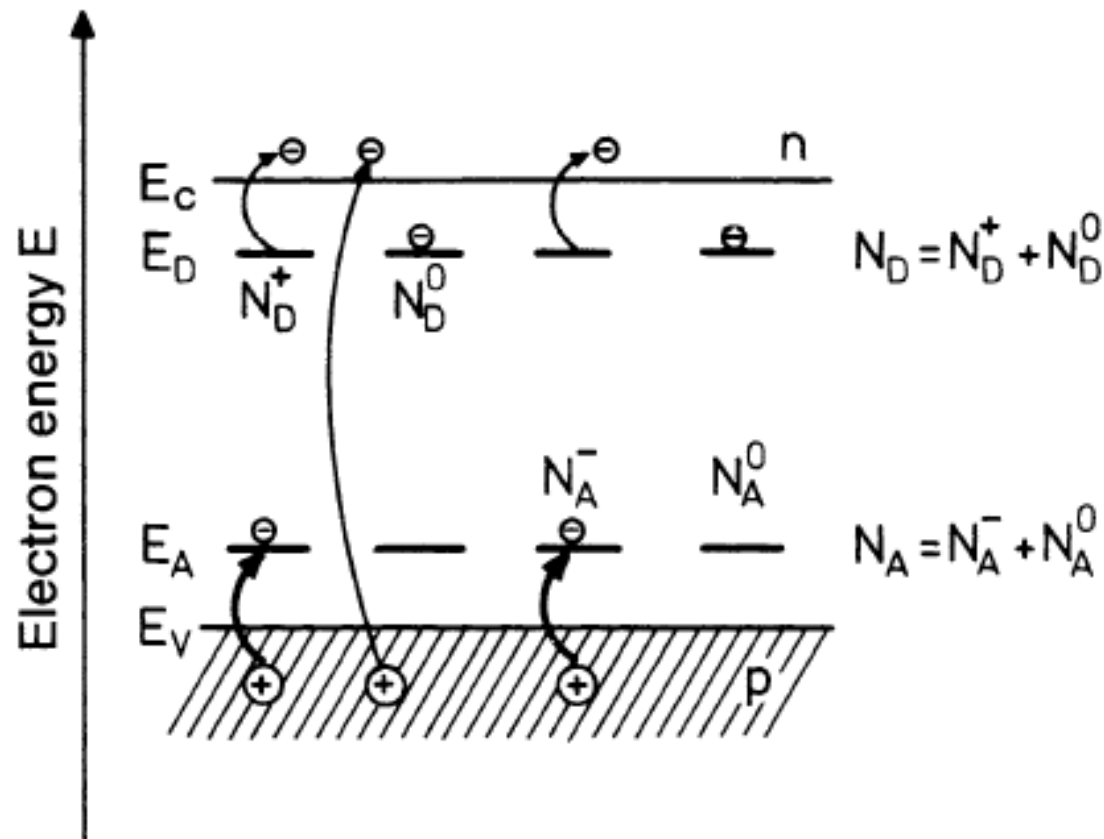
Condición de neutralidad:

$$n + N_A^- = p + N_D^+$$

La concentración de impurezas neutras a una dada temperatura esta por

$$N_D^0 = N_D [1 + \exp((E_D - \mu) / kT)]^{-1}$$

$$N_A^0 = N_A [1 + \exp((\mu - E_A) / kT)]^{-1}$$



Consideremos un semiconductor de tipo n “puro”

($N_A = 0$)

$$n = N_{\text{eff}}^{\text{C}} e^{-(E_{\text{C}} - \mu) / \epsilon T}, \quad N_{\text{eff}}^{\text{C}} = 2 \left(\frac{m_{\text{n}}^* k_{\text{B}} T}{2\pi \hbar^2} \right)^{3/2}$$

$$N_{\text{D}} = N_{\text{D}}^0 + N_{\text{D}}^+,$$

$$N_{\text{D}}^0 = N_{\text{D}} [1 + \exp((E_{\text{D}} - \mu) / \epsilon T)]^{-1}$$

μ ?

Asumiremos que la principal contribución proviene de las impurezas ionizadas $N_{\text{D}}^+ \gg n_i$ ($np = n_i^2$)

$$n \approx N_{\text{D}}^+ = N_{\text{D}} - N_{\text{D}}^0$$

$$n \approx N_{\text{D}} \left(1 - \frac{1}{1 + \exp[(E_{\text{D}} - \mu) / \epsilon T]} \right)$$

$$n = N_{\text{eff}}^{\text{C}} \exp\left(-\frac{E_{\text{C}} - \mu}{kT}\right) \longrightarrow (n/N_{\text{eff}}^{\text{C}})e^{E_{\text{C}}/kT} = e^{\mu/kT}$$

$$n \approx \frac{N_{\text{D}}}{1 + e^{E_{\text{d}}/kT} n/N_{\text{eff}}^{\text{C}}} \quad \text{donde} \quad E_{\text{d}} = E_{\text{C}} - E_{\text{D}}$$

$$n + \frac{n^2}{N_{\text{eff}}^{\text{C}}} e^{E_{\text{d}}/kT} \approx N_{\text{D}}$$

La solución con sentido físico es:

$$n \approx 2N_{\text{D}} \left(1 + \sqrt{1 + 4 \frac{N_{\text{D}}}{N_{\text{eff}}^{\text{C}}} e^{E_{\text{d}}/kT}} \right)^{-1}$$

- Si la temperatura es tan baja que

$$4(N_D/N_{\text{eff}}^L)e^{E_d/2kT} \gg 1 \quad \Rightarrow \quad n \approx \sqrt{N_D N_{\text{eff}}^C} e^{-E_d/2kT}$$

- Si la temperatura es tal que

$$4(N_D/N_{\text{eff}}^C)e^{E_d/2kT} \ll 1 \quad \Rightarrow \quad n \approx N_D = \text{const}$$

- Si la temperatura es muy alta

$$n = \cancel{N_D^+} + p \quad \Rightarrow \quad n_i = p_i = \sqrt{N_{\text{eff}}^C N_{\text{eff}}^V} e^{-E_g/2kT}$$

