SEMICONDUCTORS PHYSICS

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Objectives

- To Understand the interest of semiconductors in the production of electronic components
- To Understand transport mechanisms and physical processes governing the operation of electronics devices.
- Mastering DC and AC operations of the basic PN junction
- To Have all the basics to understand the behavior of electronic active devices

Plan

1. Crystal structure and crystallography
2. Quantum / wave mechanics: the Schrödinger equation
3. Quasi free electrons: the Sommerfeld model
4. The electrons in a periodic structure: Bloch – Brillouin model
5. Current in solids and case of semiconductors
6. Statistical mechanics: the Fermi Dirac function and approximation of Maxwell - Boltzmann
7. Semiconductor at equilibrium
8. Doping of semiconductor
9. Semiconductor at nonequilibrium: currents in the semiconductor
10. PN junction

bibliography

- C. Kittel, « physique de l'état solide », dunod université, 5° ed., 1983
- H. Mathieu, « Physique des semiconducteurs et des composants électroniques », dunod, 5° ed., 2004
- J. Singh, « physics of semiconductors and their heterostructures »,Mc.Graw Hill, 1993
- D.A.Neamen, « semiconductor physics and devices: basic principles », Mc.Graw Hill, 2003
- Chenming C. Hu , « Modern Semiconductor Devices for Integrated Circuits », 2009
- Cours de Physique des semiconducteurs, Pr. Rouzeyre, Université de Montpellier II, 1985
- McMurry and Fay, « Chemistry », Prentice Hall; 4th edition (April 7, 2003) (les figures du chapitre 1 proviennent majoritairement de cet ouvrage)

CHAPTER 1

Crystal bonding and crystallography

Crystal structure and crystallography

- Crystalline and amorphous states
- Crystalline bonds
- Geometry of the crystals
- Crystal diffraction - Reciprocal Lattice

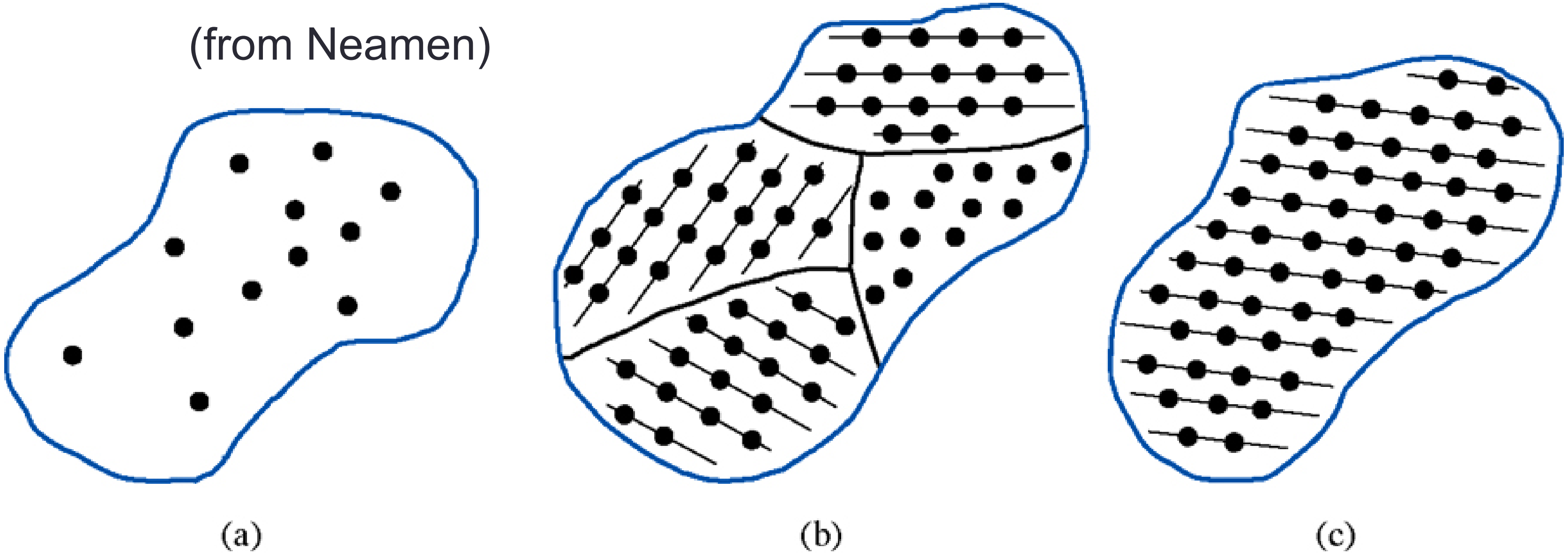
Amorphous and crystal states

- amorphous ⇔ glass
- crystal ⇔ quartz, SiO_2

- distinction:
  - At the macroscopic level:
    - If the glass temperature is raised, there is a gradual transition from the solid to the liquid state without bearing condition.
    - For a crystal, there is a temperature plateau caused by coexistence (change) phase.
  - At the microscopic level:
    - Amorphous: random distribution of the atoms
    - Crystal: spatial periodic distribution of atoms.

Amorphous and crystal states

(from Neamen)



Amorphous
(no order)

Polycrystalline
(order over many atomic dimensions)

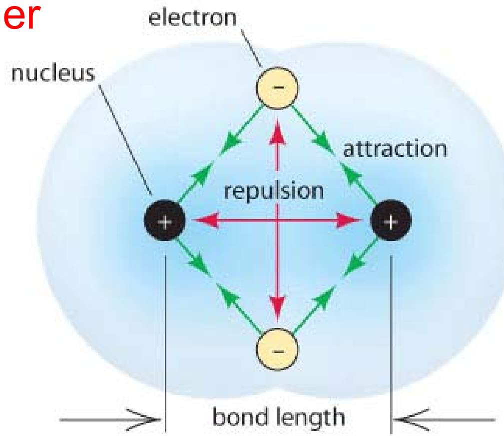
Single Crystal
(high degree of order)

Crystal bond

- What are the strengths that allow atoms bond together and form such structures?

The idea : $U_{crystal} - U_{free} < 0$

- Several parameters / considerations to take onto account:
  - Keep the positively charged ions away from each other
  - Keep the negatively charged electrons away from each other
  - Keep the electrons close to the ion
  - Minimize the kinetic energy of electrons by spreading

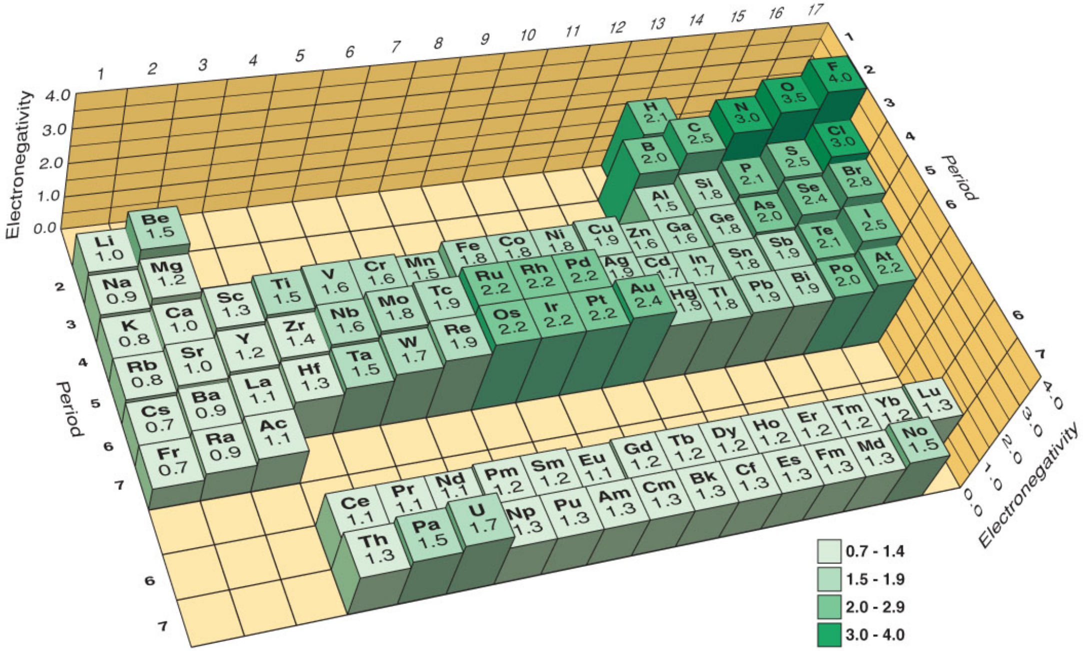


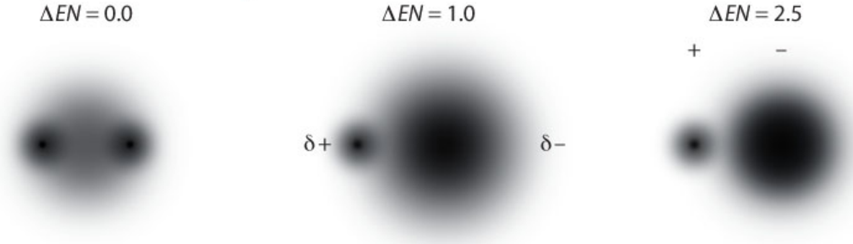
Electronegativity

- **Electronegativity:** it is the ability of an atom to attract electrons shared in a covalent bond.

The electronegativity ΔEn between two bonded atoms could be null, low or high.

•ΔEN ~ 0: the electrons are equally distributed
•ΔEN ~ 1: electrons are closest to the most electronegative atom.
•ΔEN is high, the electrons are not shared





Crystal bond

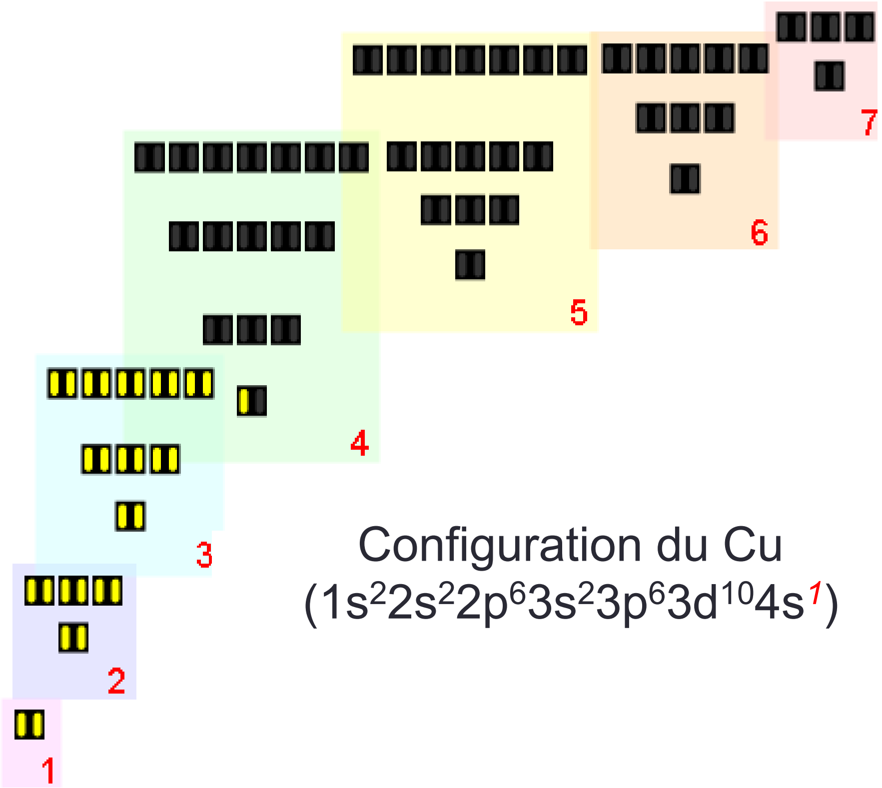
- 4 differents types:
  - metal
  - covalent
  - ionic
  - Van der Waals (noble gaz) or molecular

- One commun point:
  - Atoms try to have their last electronic layer empty or full !

Metallic bond

- Most chemical elements have a more or less pronounced metallic behavior.
- Built up from elements with few valence electrons compared to their period or energy level
- Example:
    - Sodium (Na) ⇔ $1s^2 2s^2 2p^6 3s^{1}$
    - Cuivre (Cu)⇔ $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^{1}$

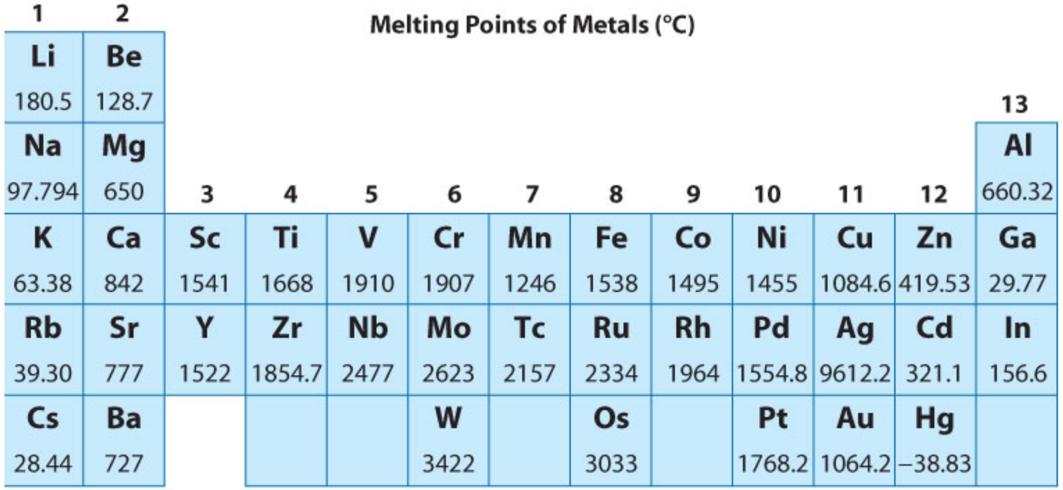
Metallic bond: copper



Configuration du Cu
($1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$)

Metallic bond

- Outers electrons not strongly linked to atom
- Tis atom can « free » this (these) electron (s)
- nucleus+core electrons look like to a set of positives charges ⇔ positive ions with saturated outer layer
- The cohesion is ensured by the negatively charged electron cloud
- Bonding's force⇔ Coulomb attraction
- Weak bonds⇔ softer materials and low melting temperature

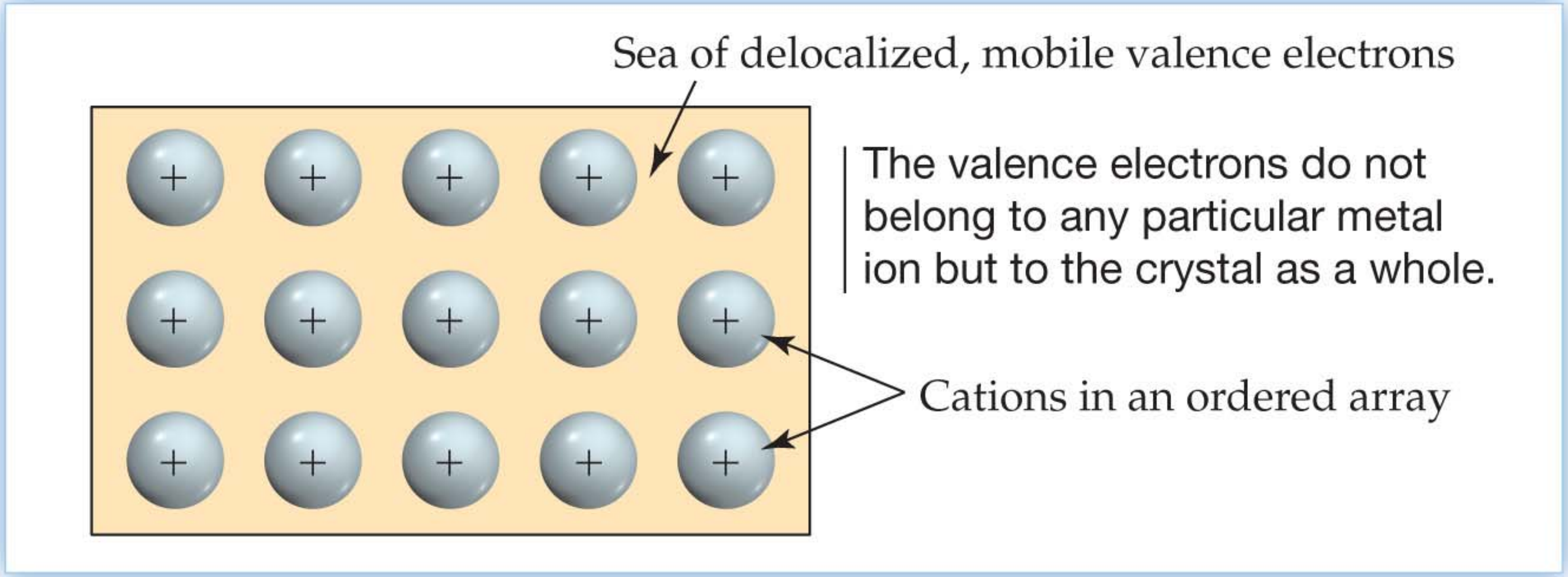


Melting Points of Metals (°C)

1	2	3	4	5	6	7	8	9	10	11	12	13
Li 180.5	**Be** 128.7											
Na 97.794	**Mg** 650											**Al** 660.32
K 63.38	**Ca** 842	**Sc** 1541	**Ti** 1668	**V** 1910	**Cr** 1907	**Mn** 1246	**Fe** 1538	**Co** 1495	**Ni** 1455	**Cu** 1084.6	**Zn** 419.53	**Ga** 29.77
Rb 39.30	**Sr** 777	**Y** 1522	**Zr** 1854.7	**Nb** 2477	**Mo** 2623	**Tc** 2157	**Ru** 2334	**Rh** 1964	**Pd** 1554.8	**Ag** 9612.2	**Cd** 321.1	**In** 156.6
Cs 28.44	**Ba** 727				**W** 3422		**Os** 3033		**Pt** 1768.2	**Au** 1064.2	**Hg** −38.83	

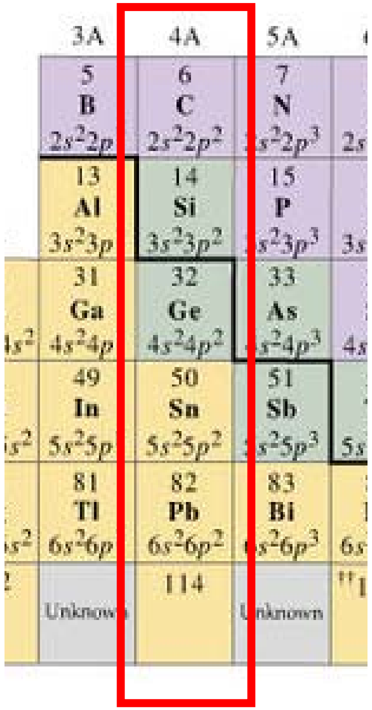
Metallic bond

Electron-Sea Model: A metal crystal is viewed as a three-dimensional array of metal cations immersed in a sea of delocalized electrons that are free to move throughout the crystal.

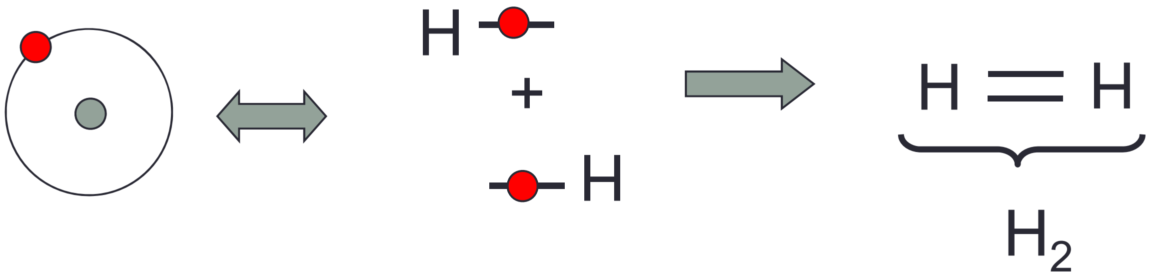


Covalent bond

- Crystals belong to column IV of periodic table
- Hydrogen like bonds
- Hydrogen:
  - 1 outer electron
  - To complete the layer, try to « find, accept » an extra electron
  - A second electron from another Hydrogen will allow to share outer electrons
  - We get H_2 molecule

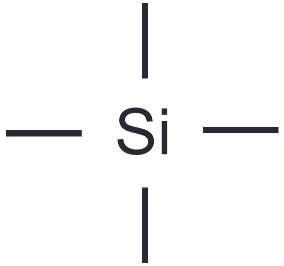


3A	4A	5A
5 B $2s^22p$	6 C $2s^22p^2$	7 N s^22p^3
13 Al $3s^23p$	14 Si $3s^23p^2$	15 P s^23p^3
31 Ga $4s^24p$	32 Ge $4s^24p^2$	33 As s^24p^3
49 In $5s^25p$	50 Sn $5s^25p^2$	51 Sb s^25p^3
81 Tl $6s^26p$	82 Pb $6s^26p^2$	83 Bi s^26p^3
Unknown	114	nknown

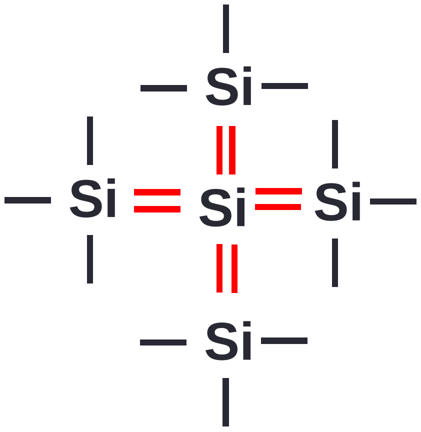


Covalent bond

- Example : Silicon
  - 4 valence (outer) electrons



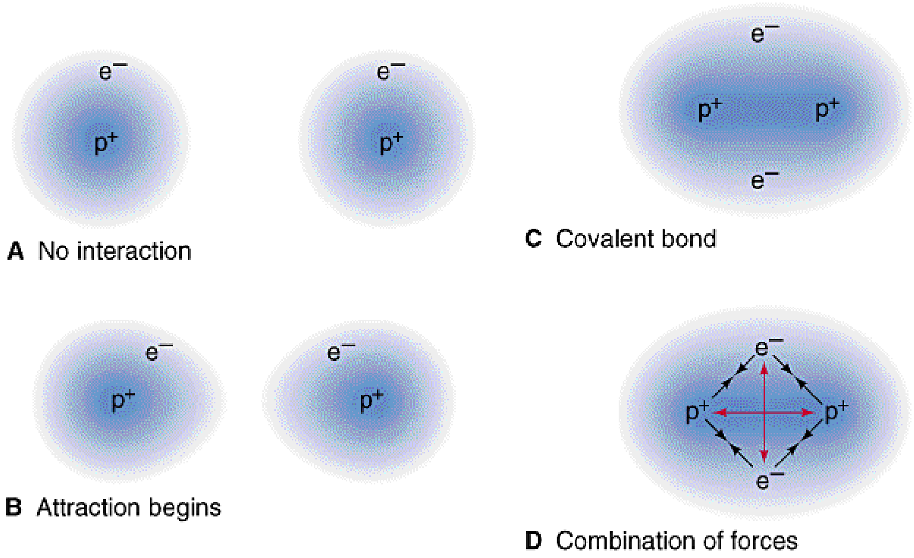
  - Need four more electrons to complete the valence energy shell
  - It is sufficient to bring four other Silicon



A significant difference between the covalent bonding of Hydrogen and Silicon: Unlike H2, once saturated links, the other four still have Silicon "dangling" bonds ⇔ This process may continue ⇔ then we form a crystal.

Covalent bond

- Lower energy if the electrons wander near the 2 nucleus
- We can get the same result with II-VI or III-V compounds (see after)

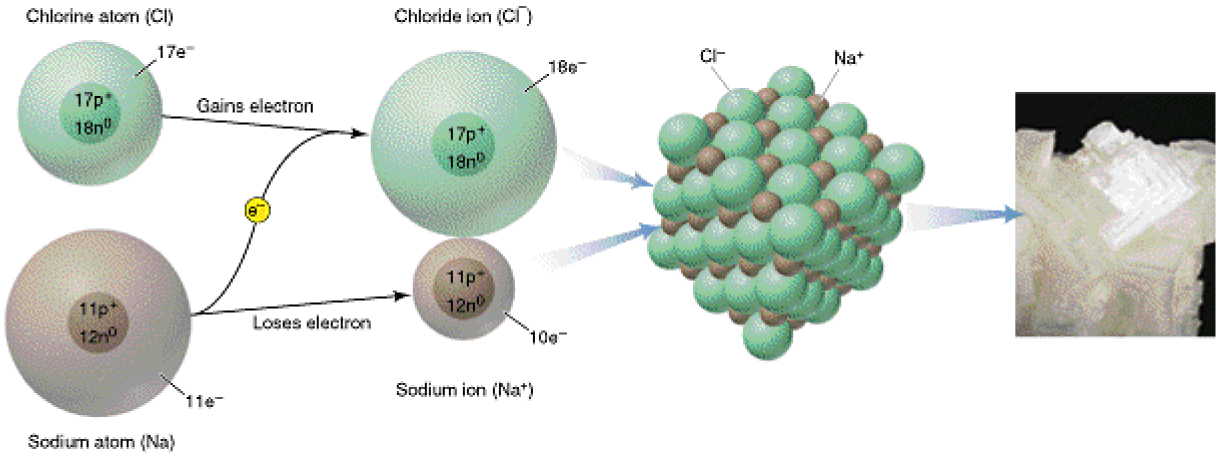


Ionic bond

- Association of a strongly electronegative chemical element (7e) and a strongly electropositive element (1e): ex NaCl
- The elements in group 1 of the periodic table tend to lose their one electron (become positively charged) while the elements in group VII gain one electron and become negatively charged $\Leftrightarrow$ the two ions experience coulomb attraction

$3s^2 3p^5$

$3s^1$



A Electron transfer **B** Arrangement of Na^+ and Cl^- in a crystal **C** Sodium chloride crystal

(D'après McMurry and Fay)

Ionic bond

- The strengh of cohesion is due to the Coulomb attraction of the two ions ⬄ ionic bond
- In fact, binding is "identical" to the covalent bond except that atoms are very differents (not the same column)
- Ionic/covalent border is not sharp: depends on the electronic nature of the associated elements Col I – VII ⬄ mainly ionic
  - Col II-VI ⬄ 80% ionic 20% covalent (CdTe)
  - Col III-V ⬄ 60% ionic 40% covalent (GaAs, GaP, InP)
  - Col IV-IV ⬄ essentielly covalent (Si, Ge)

Ionic bond

- the electron released from alcali meal (Na) is trapped by the halogen (Cl)
- None electron released in the lattice
- Ionic crystals are generally insulating
- Bonds between atom very strong ⇔ very hard crystals

Van der Waals bond

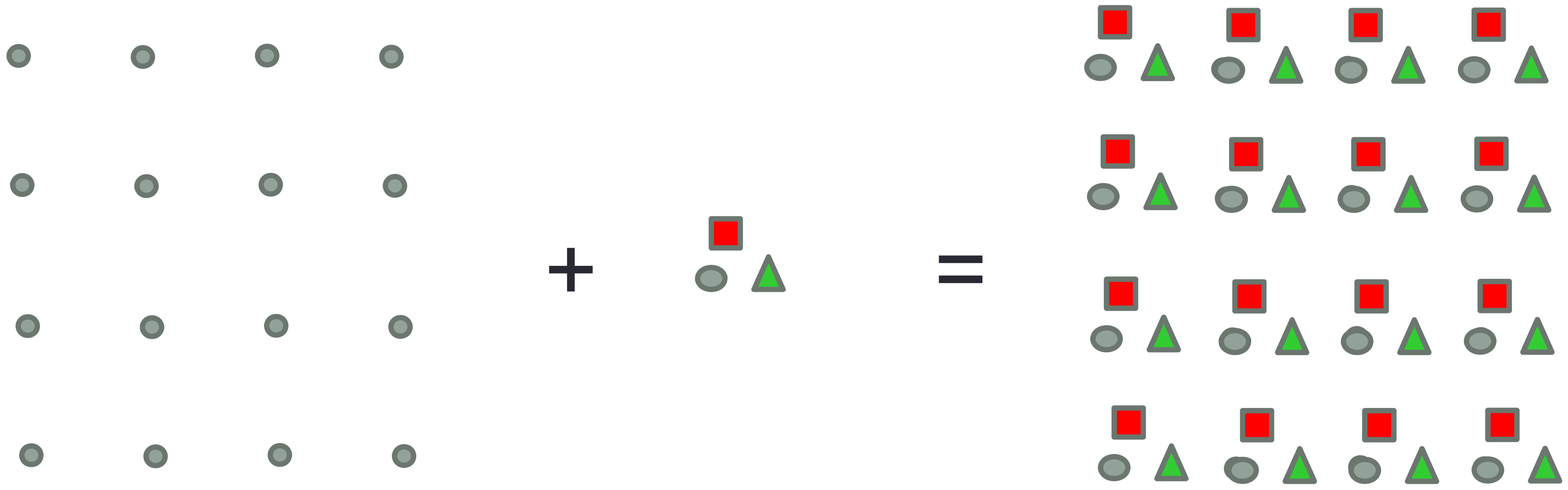
- Weakest of the chemical bonds
- Electronic distribution = free atom
- Most of this materials are in gazeous form at RT
- Electronics shells (layers) already saturated (col. VIII)
- Very weak binding energy (few% of the ionization energy of the atom) ⇔ crystals melt at low temperature
- Responsible for the cohesion of the molecules

Crystal geometry

- The building block which is repeated infinitely, to produce the crysal,may be a single atom or quite complex (protein) : this is the basis.
  - For Si,Ge basis : one atom
  - For GaAs basis : 2 atoms
  - For molecular atom basis : Protein 10^4-10^5 at.!!

- The lattice represents a set of points in space which form a periodic structure
- 2 Dim: net (Réticule)
- 3 Dim: Lattice (Réseau)

Crystal geometry



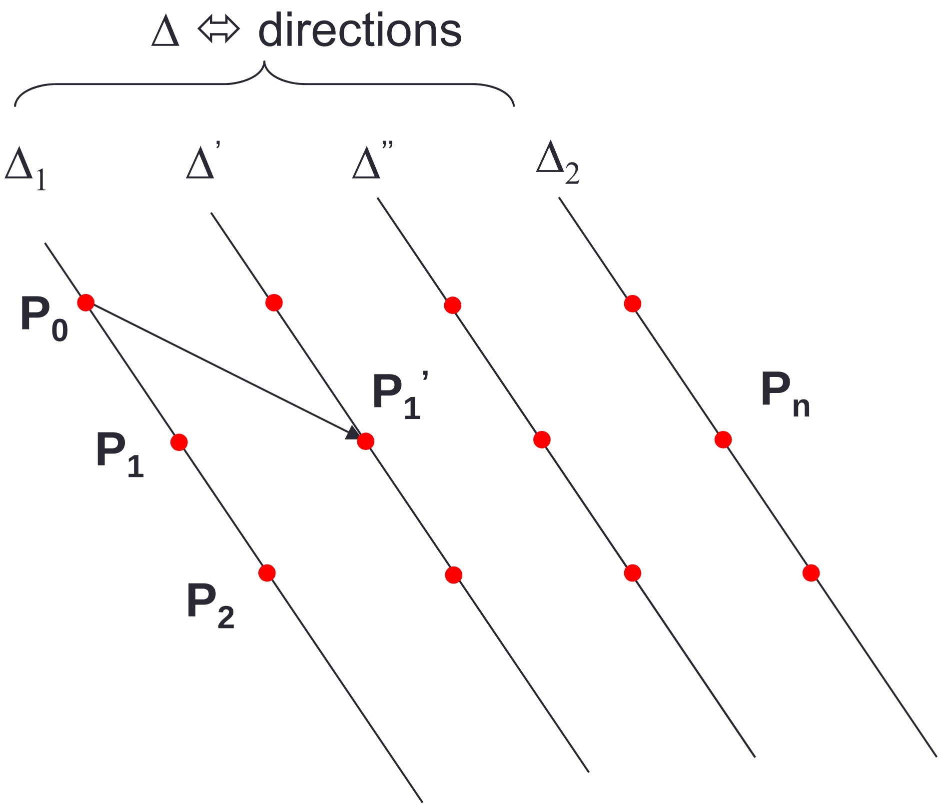
Lattice
(réseau)

Basis (base):
a builing block of atoms

Crystal structure
(structure cristalline)

Crystal geometry

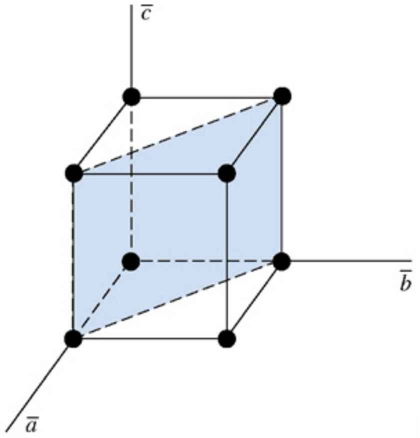
- Bravais Postulat : it exists in the crystal a set of points Pn with exactly the same microscopic environment that P0 (origin pt) *ie* that the atomic landscape seen from Pn is the same as P0 in magnitude and direction. This set of points is a set of congruent points or vertex (top) of the lattice
- Bravais lattice: it is a sample of the lattice that shows all the translations of the lattice. There are 14 different lattices



Notation to denote planes and points in a lattice: Miller indices

- Lattice planes: the points (nœuds) of the lattice can be grouped on sets of parallel and equidistant planes : reticular planes (les plans réticulaires)

- Method :
  - Take the intercepts of the plane along the axis
    - x_1 (distance / origin = $x_1.a$) in units of lattice constant a
    - x_2 (distance / origin = $x_2.b$) in units of lattice constant b
    - x_3 (distance / origin = $x_3.c$ in units of lattice constant c
  - Take the reciprocal of the intercepts
  - Reduce them to the smallest integers (in the same ratio !)
  - We get the Miller indices
  - Example:
    - $x_1=4$, $x_2=1$, $x_3=2$
    - ¼ , 1, ½
    - 1,4,2 (h,k,l) =(1,4,2)

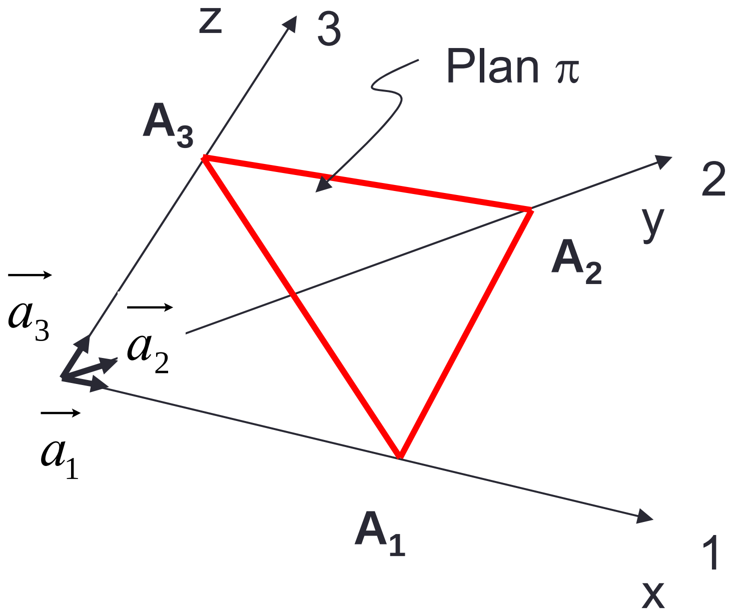


(b)

  - Nota : in case of negative number, we place a minus sign over $\bar{h}$

  - (h,k,l) defines a plane

Crystalline planes (h,k,l)



- A_1, A_2, A_3 : 3 nodes ⇔ reticular plane π. $\overline{OA_i} = p_i \overline{a_i}$
- consider M($\overline{OM} = x_1\overline{a_1} + x_2\overline{a_2} + x_3\overline{a_3}$) point of direct lattice
- π plane can be described by : $hx + ky + lz = N$
- It can be rewritten:

$$\frac{x}{p_1} + \frac{y}{p_2} + \frac{z}{p_3} = 1$$

Using Miller index, we get : $hx + ky + lz = N$. If N=2, π plane is the second plane (h,k,l) after origin.

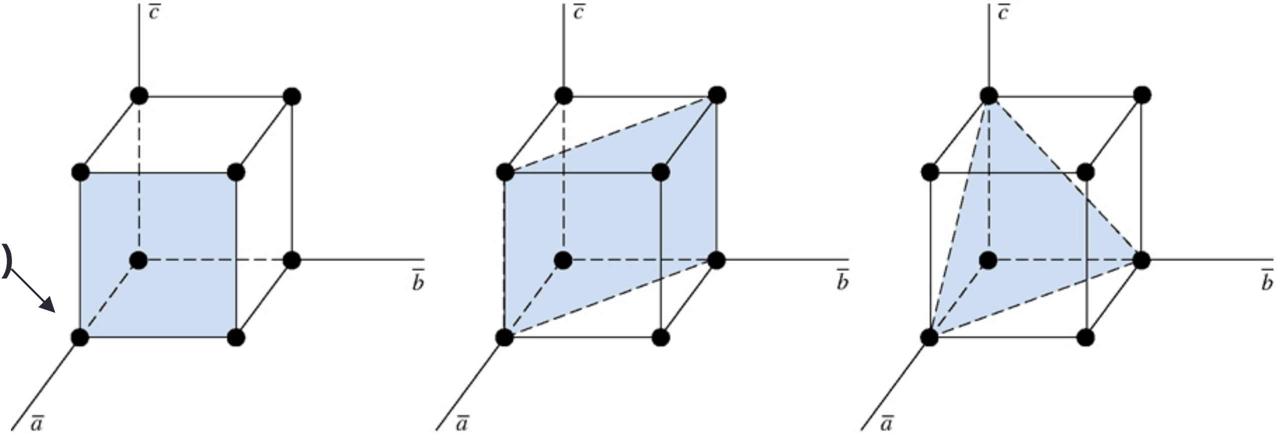
Crystallographic direction

- Any line through two points of the lattice defines a crystallographic direction. It's defined by 3 indices h,k,l smallest integers having the same relationship to each other that the components of a vector collinear to the line.
- Notation: [h,k,l]
- Paricular cases : one direction [h,k,l] is orthogonal to the plane of same indexes (h,k,l) or [h,k,l] is the axial vector of the plane (h,k,l) .

Miller Indices (continued)

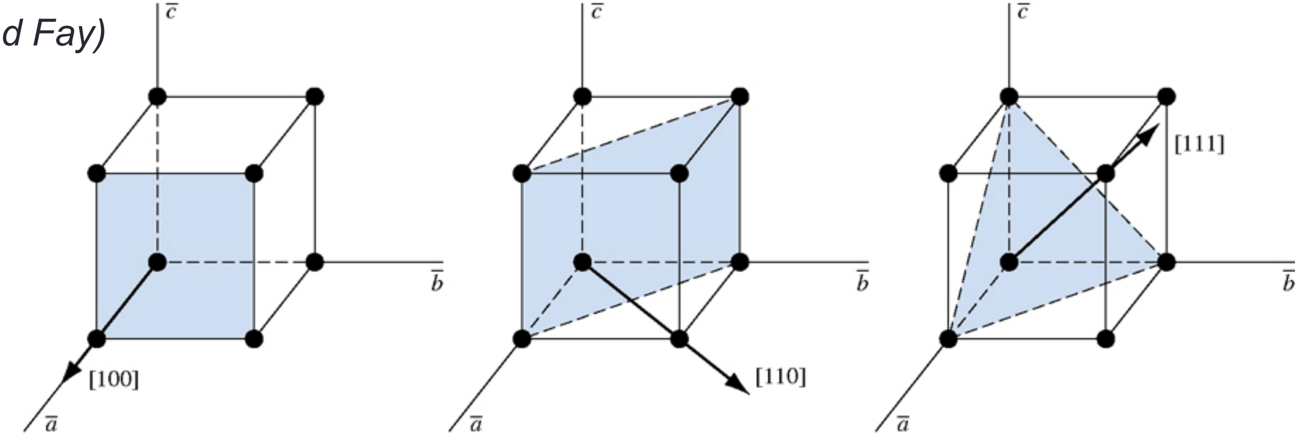
- Allow us to define crystal directions and crystal planes:

(a,0,0) ou (1,0,0)



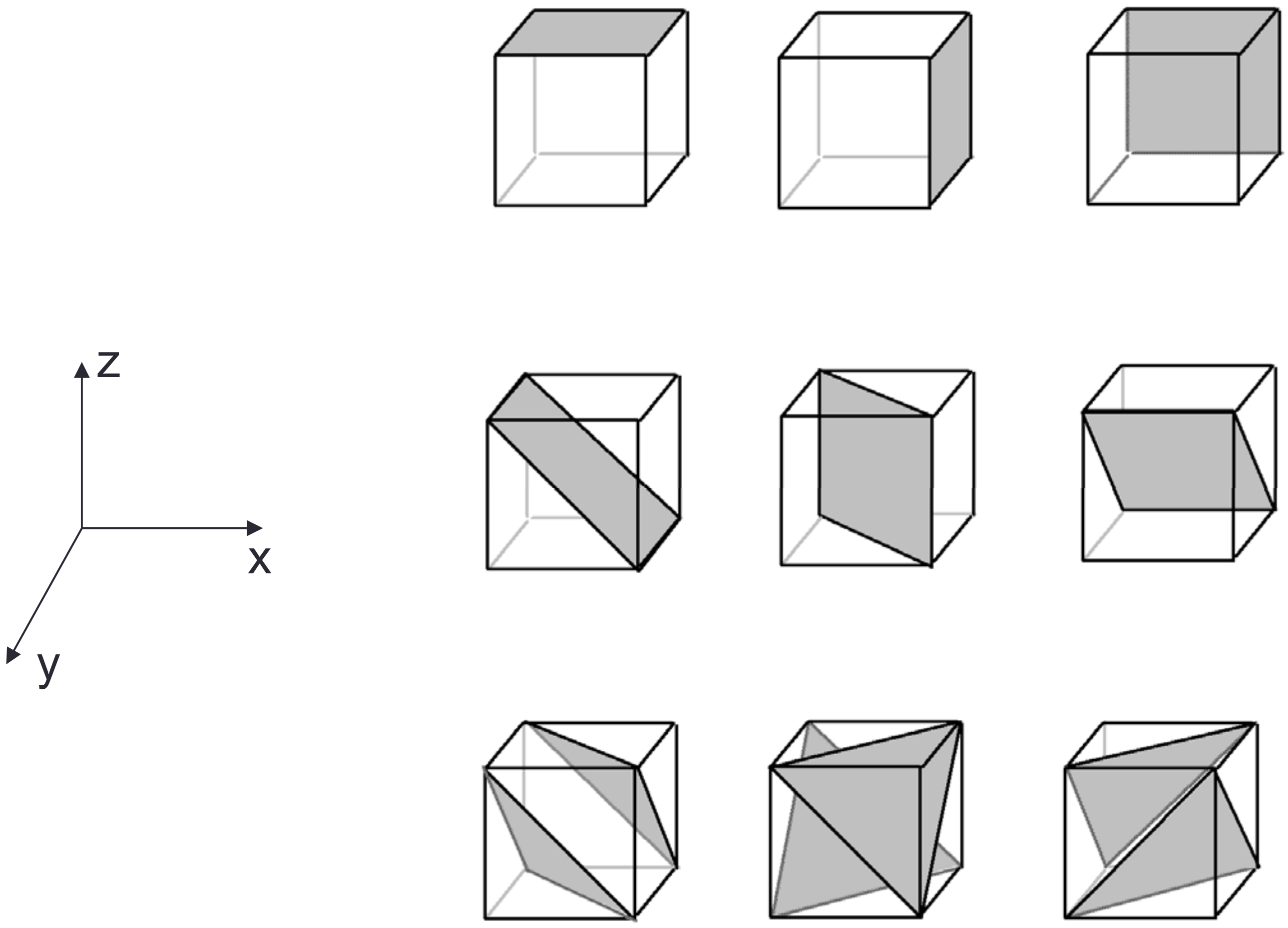
(a) (b) (c)

(From McMurry and Fay)



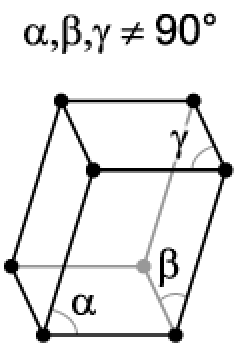
(a) (b) (c)

Some examples.

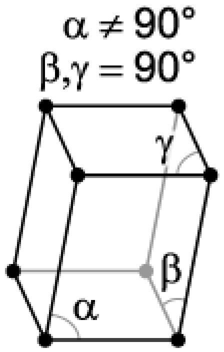


(From McMurry and Fay)

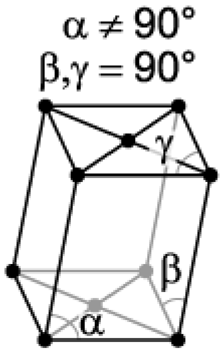
The 14 Bravais lattices in three dimensional system



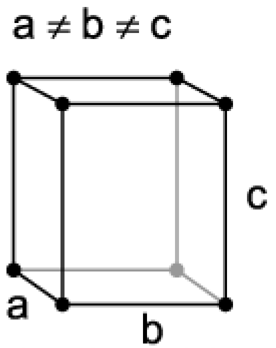
Triclinic



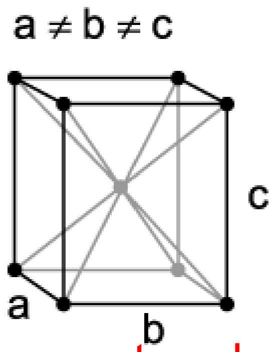
Monoclinic



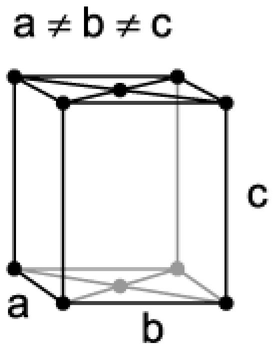
centered Monoclinic



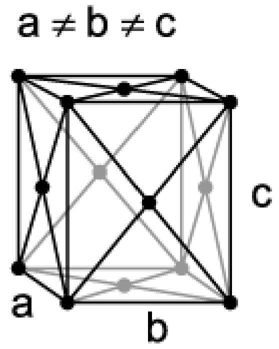
Orthorhombic



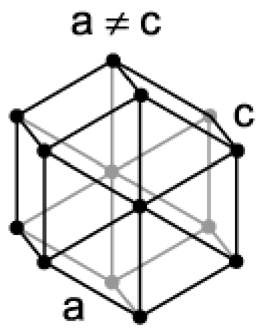
centered Orthorhombic



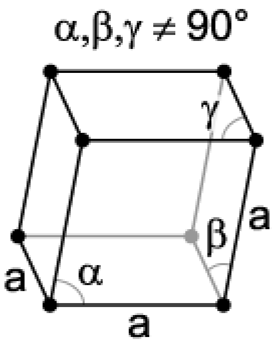
base centered Orthorhombic



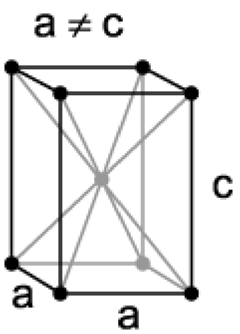
faces centered Orthorhombic



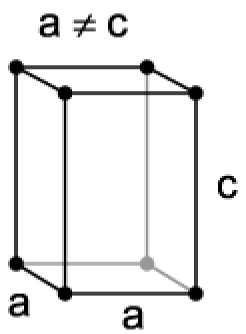
Hexagonal



Rhomboédric

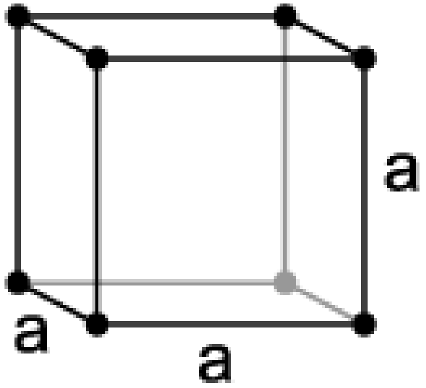


Tetragonal

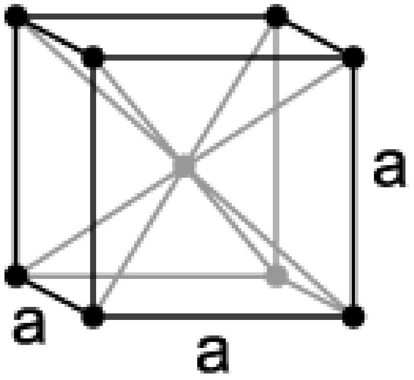


centered Tetragonal

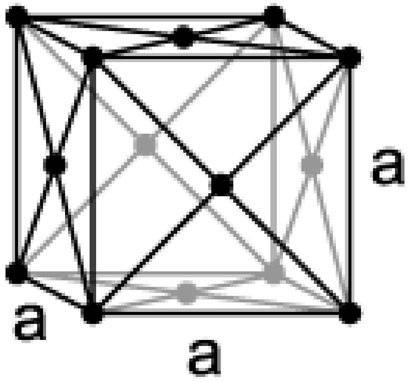
The 14 Bravais lattices in three dimensional system



Simple Cubic (sc)

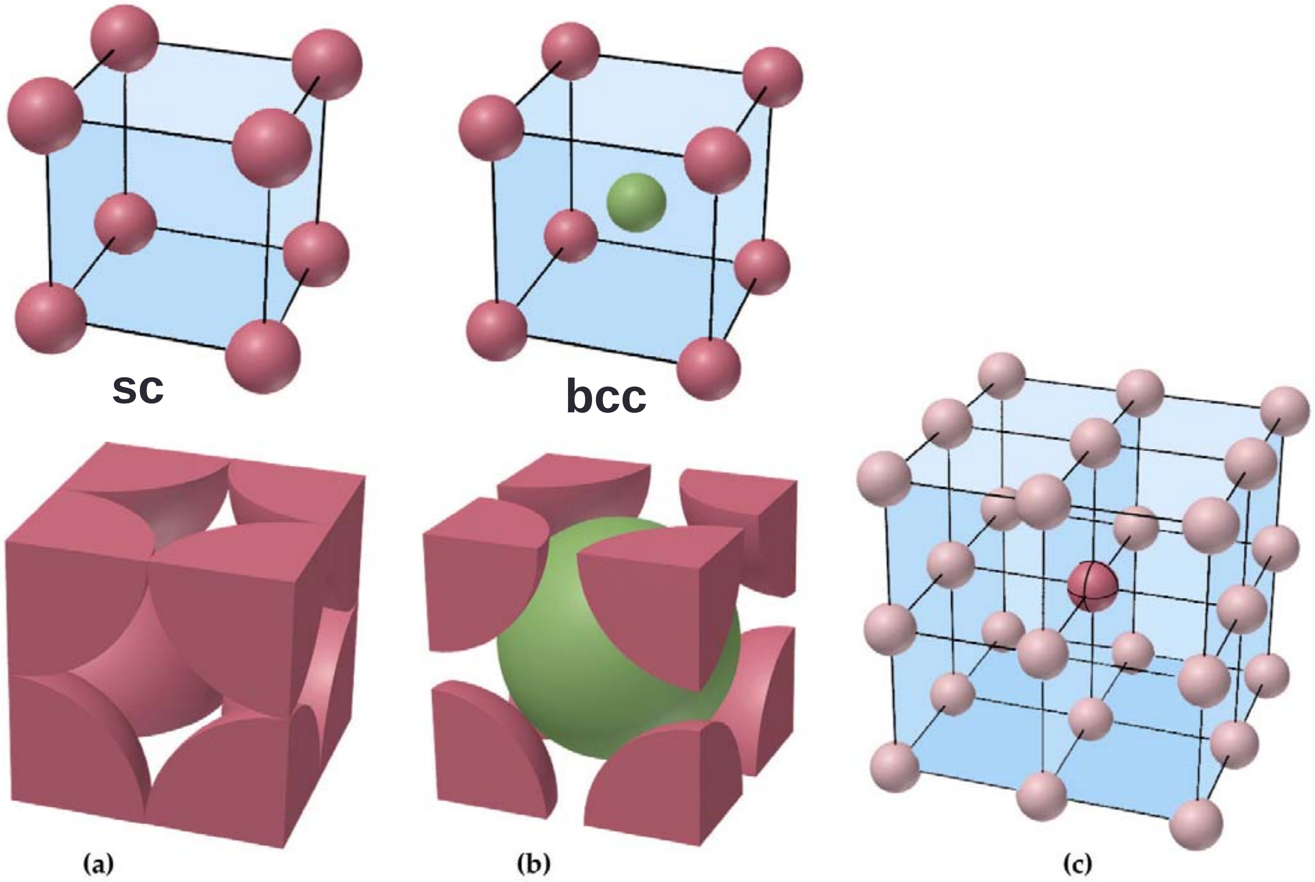


body centered (bcc) Cubic



face centered Cubic (fcc)

Crystalline structures : multiplicity of the lattice

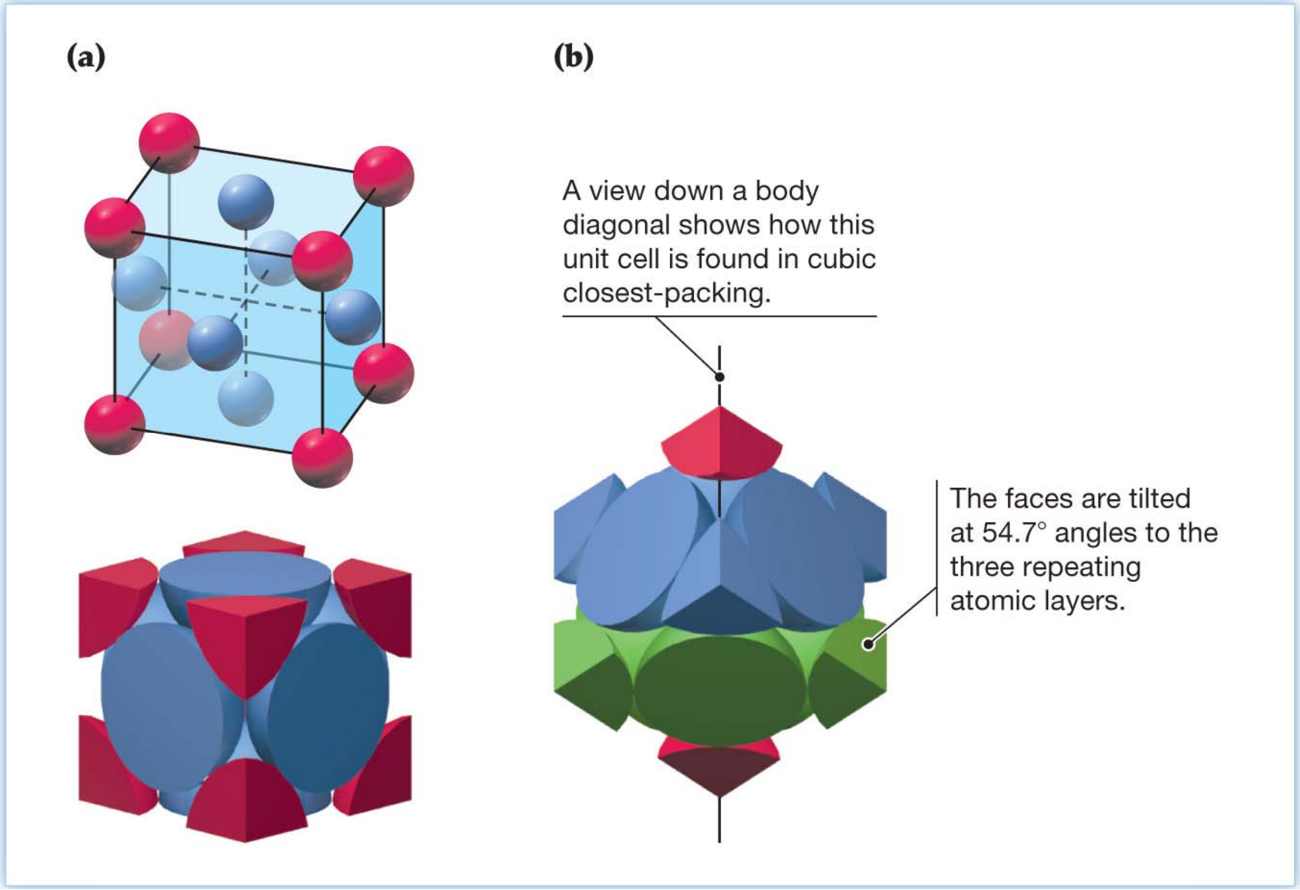


1 atom
per unit cell

2 atoms
per unit cell

(From McMurry and Fay)

Crystalline structures : multiplicity of the lattice



A view down a body diagonal shows how this unit cell is found in cubic closest-packing.

The faces are tilted at 54.7° angles to the three repeating atomic layers.

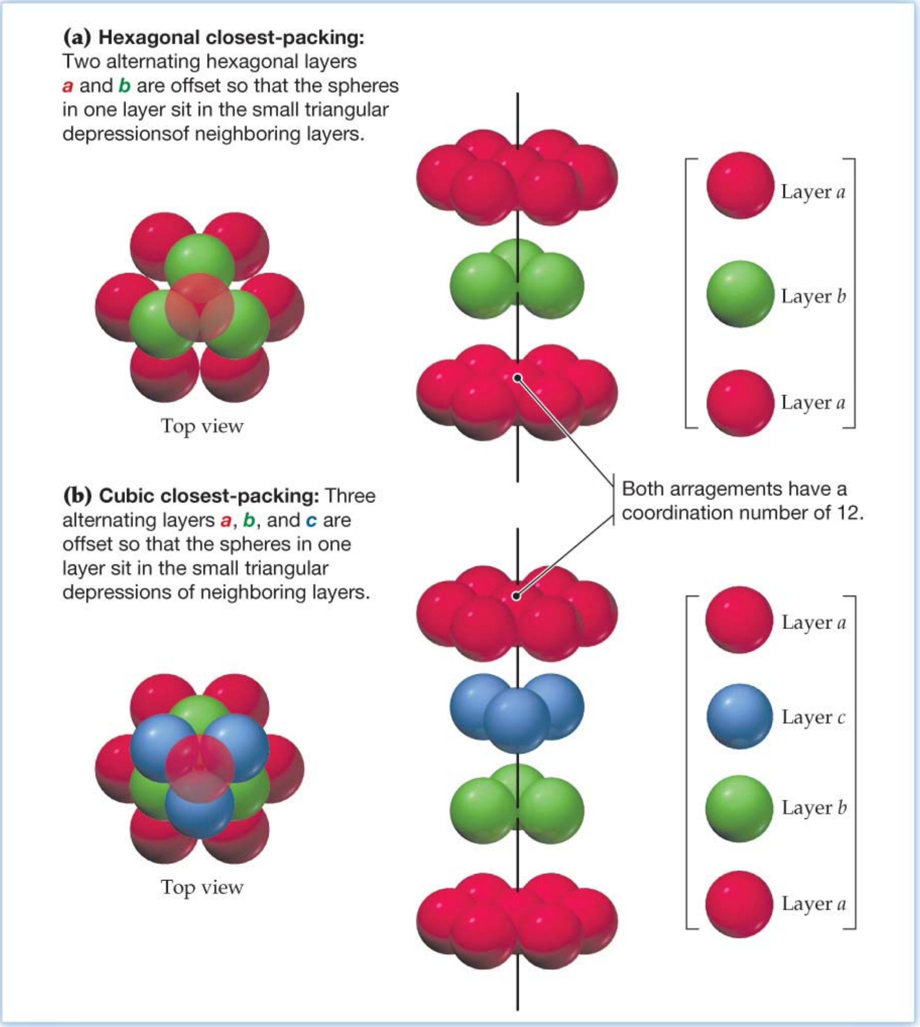
4 atoms
per unit cell

(from McMurry and Fay)

Crystalline structures : multiplicity of the lattice

Hexagonal Structure

fcc Structure



(a) Hexagonal closest-packing: Two alternating hexagonal layers *a* and *b* are offset so that the spheres in one layer sit in the small triangular depressionsof neighboring layers.

(b) Cubic closest-packing: Three alternating layers *a*, *b*, and *c* are offset so that the spheres in one layer sit in the small triangular depressions of neighboring layers.

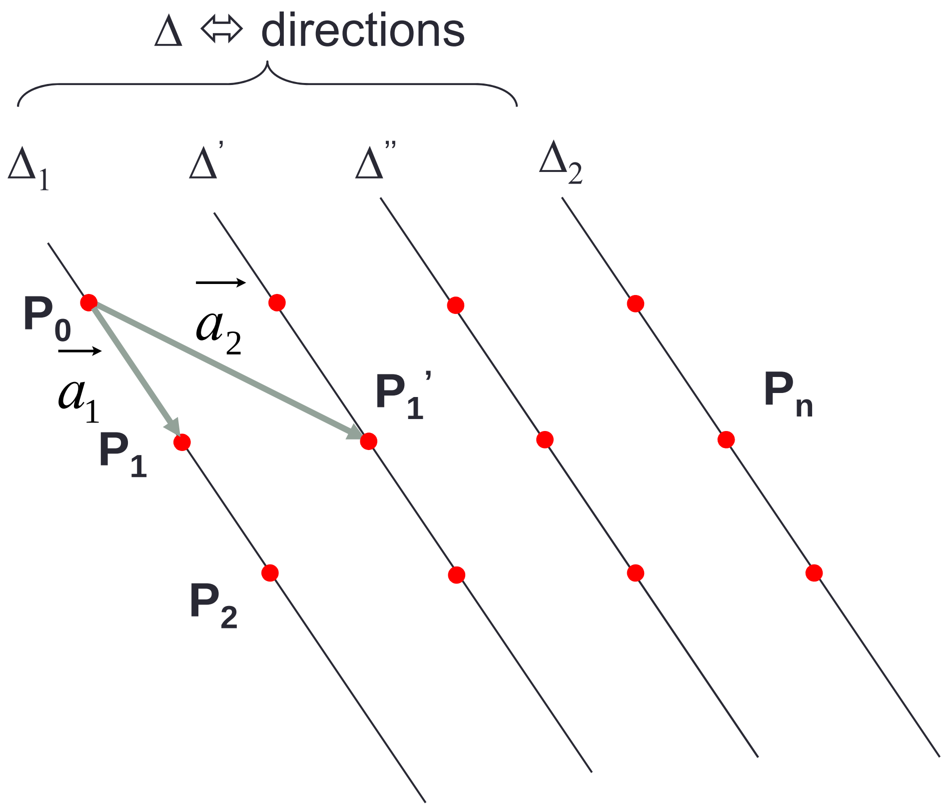
Both arragements have a coordination number of 12.

(from McMurry and Fay)

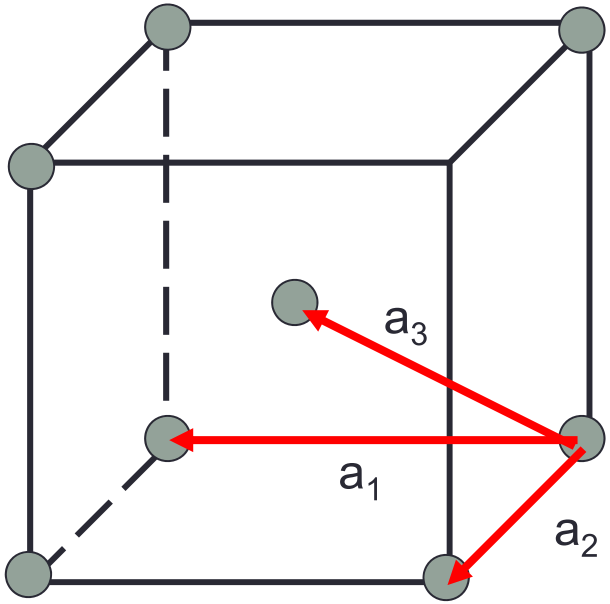
How to define the primitive unit cell

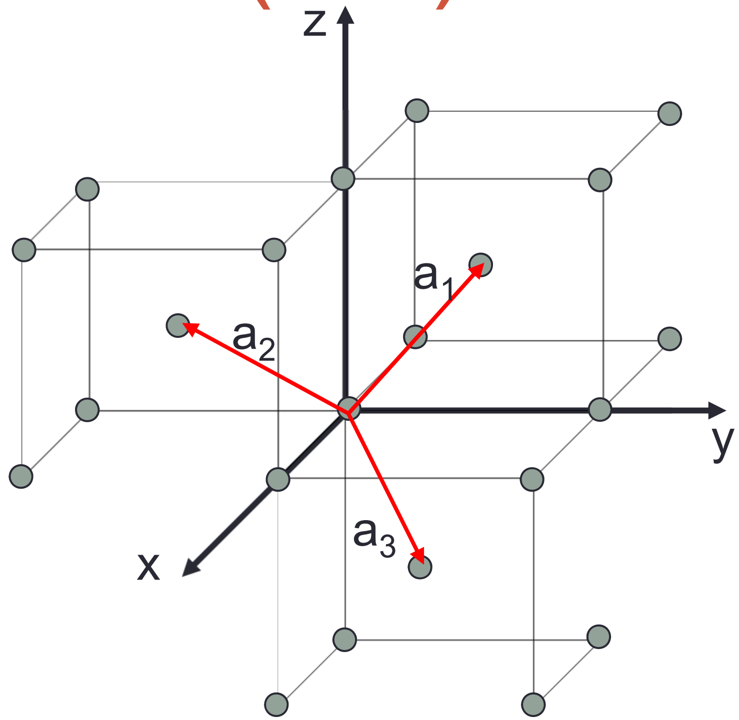
- Volume is the smallest possible
- Not unique way
- Method:
  - **a**$_1$ to be the shortest period of the lattice
  - **a**$_2$ to be the shortest period of the lattice not parallel to **a**$_1$
  - **a**$_3$ to be the shortest period of the lattice not coplanar with **a**$_1$ and **a**$_2$

⇒ *Primitive unit cell*



The body centered cubic (bcc)





$$\overrightarrow{a_1} = a\vec{x}$$

$$\overrightarrow{a_2} = a\vec{y}$$

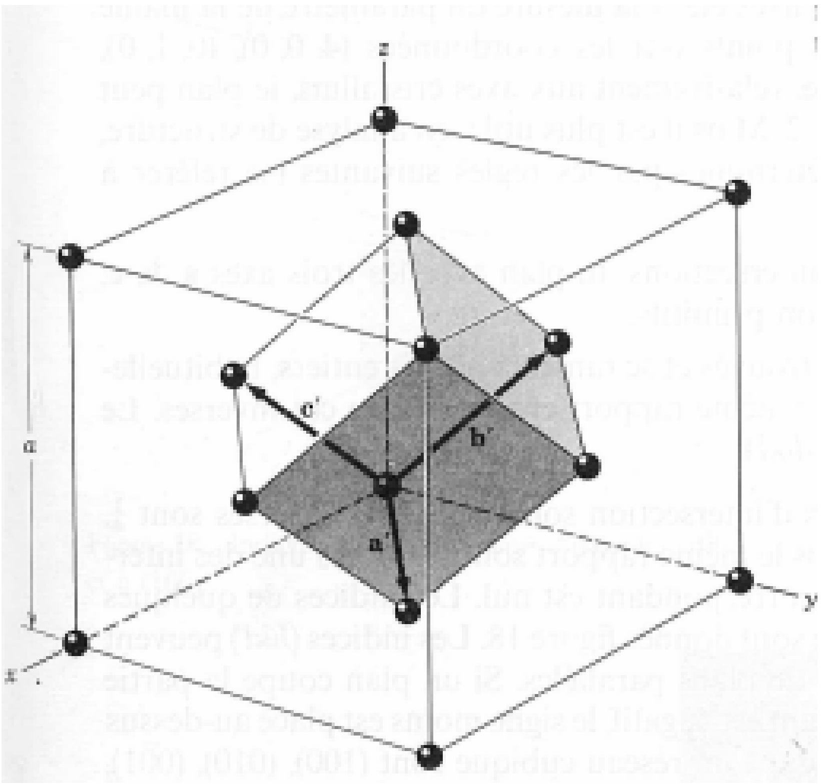
$$\overrightarrow{a_3} = \frac{a}{2}(\vec{x} + \vec{y} + \vec{z})$$

or:

$$\overrightarrow{a_1} = \frac{a}{2}(-\vec{x} + \vec{y} + \vec{z})$$

$$\overrightarrow{a_2} = \frac{a}{2}(\vec{x} - \vec{y} + \vec{z})$$

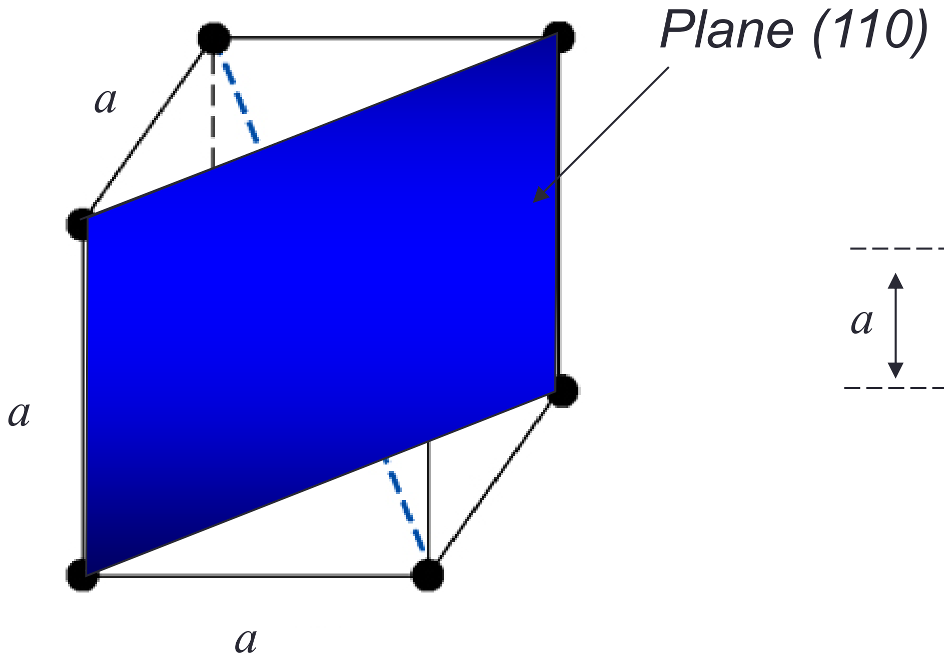
$$\overrightarrow{a_3} = \frac{a}{2}(\vec{x} + \vec{y} - \vec{z})$$

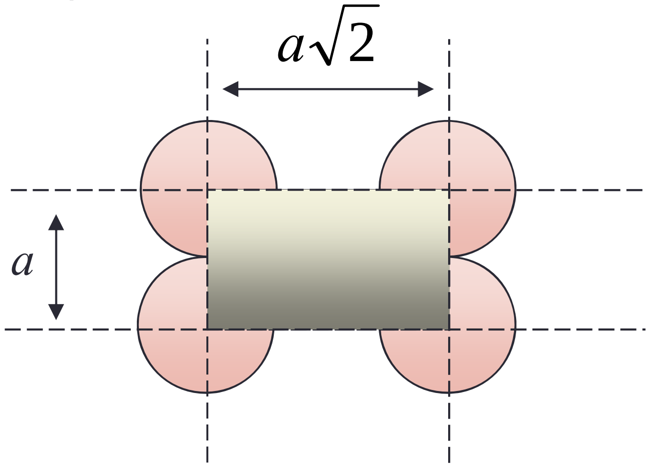


Primitive basis vectors for a fcc: the resulting lattice is a rhombohedric lattice (60° for each angle)

From C. Kittel, Dunod, 5°ed.

Atoms surface density

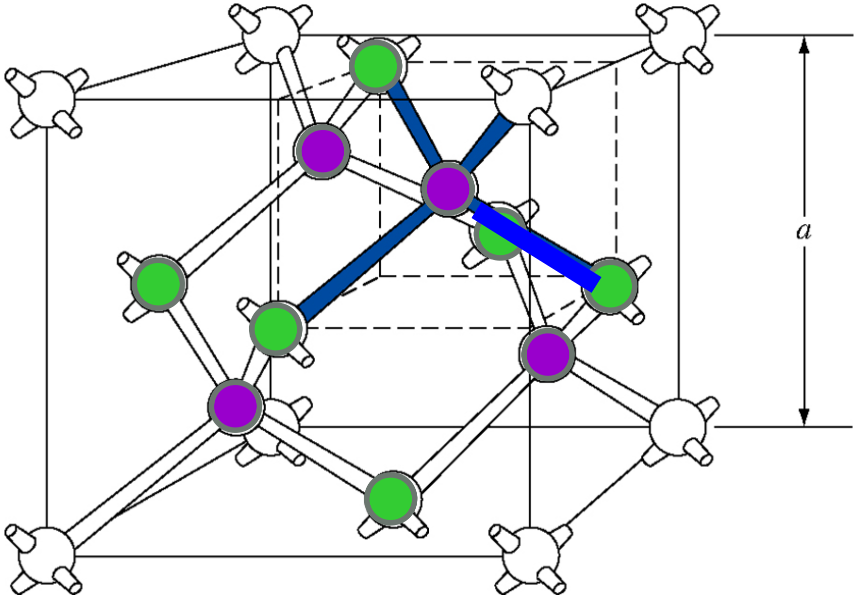




$$\text{surface density} = \frac{1+4\times 1/4}{a\times a\sqrt{2}} = \frac{2}{(5\times 10^{-8}\,cm)^2\times\sqrt{2}} = 5.66\times 10^{14}\,\text{at.}cm^{-2}$$

Silicon and its « diamond » structure

- fcc
- Two atom basis
- Looks like two fcc shifted/deplaced by ¼ diagonal
- Each atom has 4 nearest neighbors (tetragonal bond)

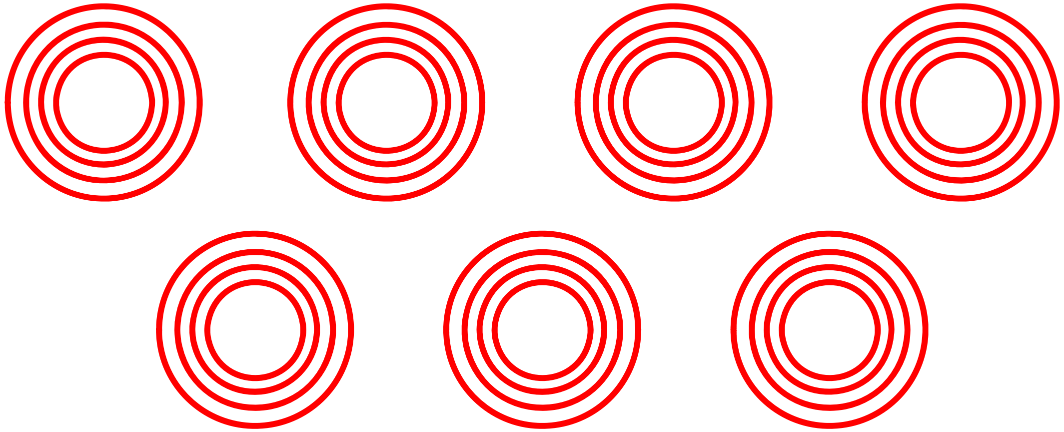


The reciprocal lattice

- *a priori*:
  - All the physical phenomena are involved in real space (3D) ⬄ real space is obviously the physical space of interest
- but:
  - For many applications/studies ⬄ most astute to work in a virtual space : reciprocal lattice.
  - Reasons: fully understood when we discuss the problem of X-ray diffraction and energy bandstructures of crystal.

The reciprocal lattice: definition

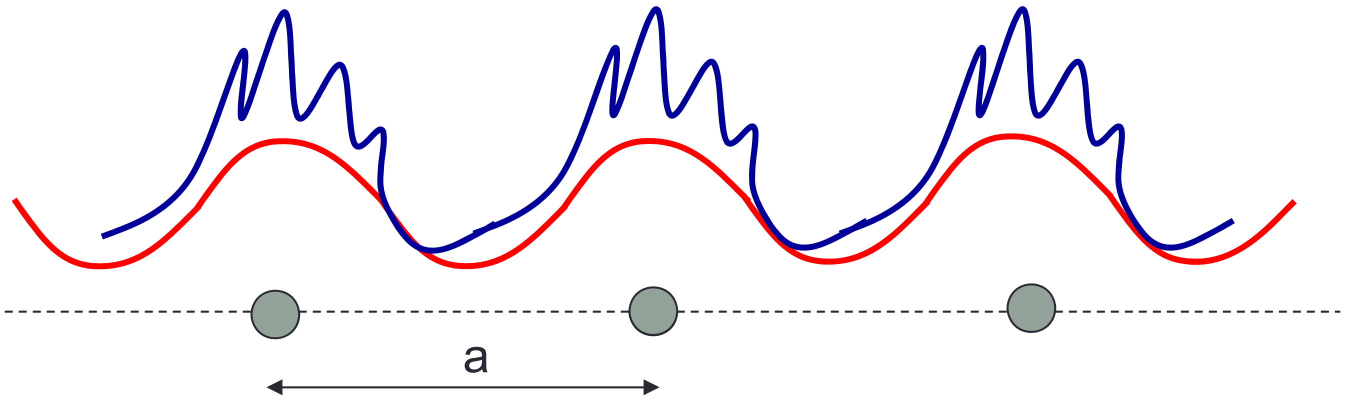
- One of the reasons of reciprocal lattice:
  - Periodic structures ⇔ physical properties likewise (local electron density, electrostatics potential, …)
  - These properties can be defined with *ad hoc* functions which are also periodic functions (crystal periodicity)



$$f(r+l) = f(r)$$

The reciprocal lattice: definition

- One dimension:
  - Structure with a period « a »



$$f(x+l)=f(x) \quad \text{avec} \quad l=l_1 a \quad l_1 \text{ entier}$$

  - Such function can be rewritten as a Fourier series

$$f(x)=\sum_n A_n e^{2\pi i n x/a}=\sum_g A_g e^{igx} \quad \text{avec } g_n=n\frac{2\pi}{a} \quad [g]=m^{-1}$$

The reciprocal lattice: definition

- verification

$$f(x)=\sum_{g} A_g e^{igx} \qquad A_g=\frac{1}{a}\int_{cellule} f(x)e^{-igx}dx$$

$$f(x+l)=\sum_{g} A_g e^{ig(x+l)} = \sum A_g e^{igx}e^{igl} = f(x) = \sum A_g e^{igx}$$

$$\Downarrow$$

$$e^{igl}=1 \Leftrightarrow gl = n\frac{2\pi}{a}l_1 a = nl_1\times 2\pi = \text{integer}\times 2\pi$$

The reciprocal lattice: definition

- We start with three primitive vectors in the real space **a**$_1$, **a**$_2$, **a**$_3$.
- We take a « simple » transformation to get three new vectors in the reciprocal lattice **b**$_1$, **b**$_2$, **b**$_3$:

$$\boxed{b_1 = 2\pi \frac{a_2 \wedge a_3}{(a_1, a_2, a_3)}} \quad \boxed{b_2 = 2\pi \frac{a_3 \wedge a_1}{(a_1, a_2, a_3)}} \quad \boxed{b_3 = 2\pi \frac{a_1 \wedge a_2}{(a_1, a_2, a_3)}}$$

$$\boxed{b_i . a_j = 2\pi\delta_{ij} \quad \text{with } \delta_{ij} = 0 \text{ if } i \neq j, \delta_{ij} = 1 \text{ if } i = j}$$

Reciprocal lattice building

- From the same origin O of the real space, we generate a reciprocal lattice.
- if N, a point of the reciprocal lattice

$$\vec{g} = \overrightarrow{ON} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

- if P, a point of the real lattice

$$\vec{l} = \overrightarrow{OP} = n\vec{a}_1 + p\vec{a}_2 + q\vec{a}_3$$

- In general Reciprocal lattice has not the same symmetries than real space lattice

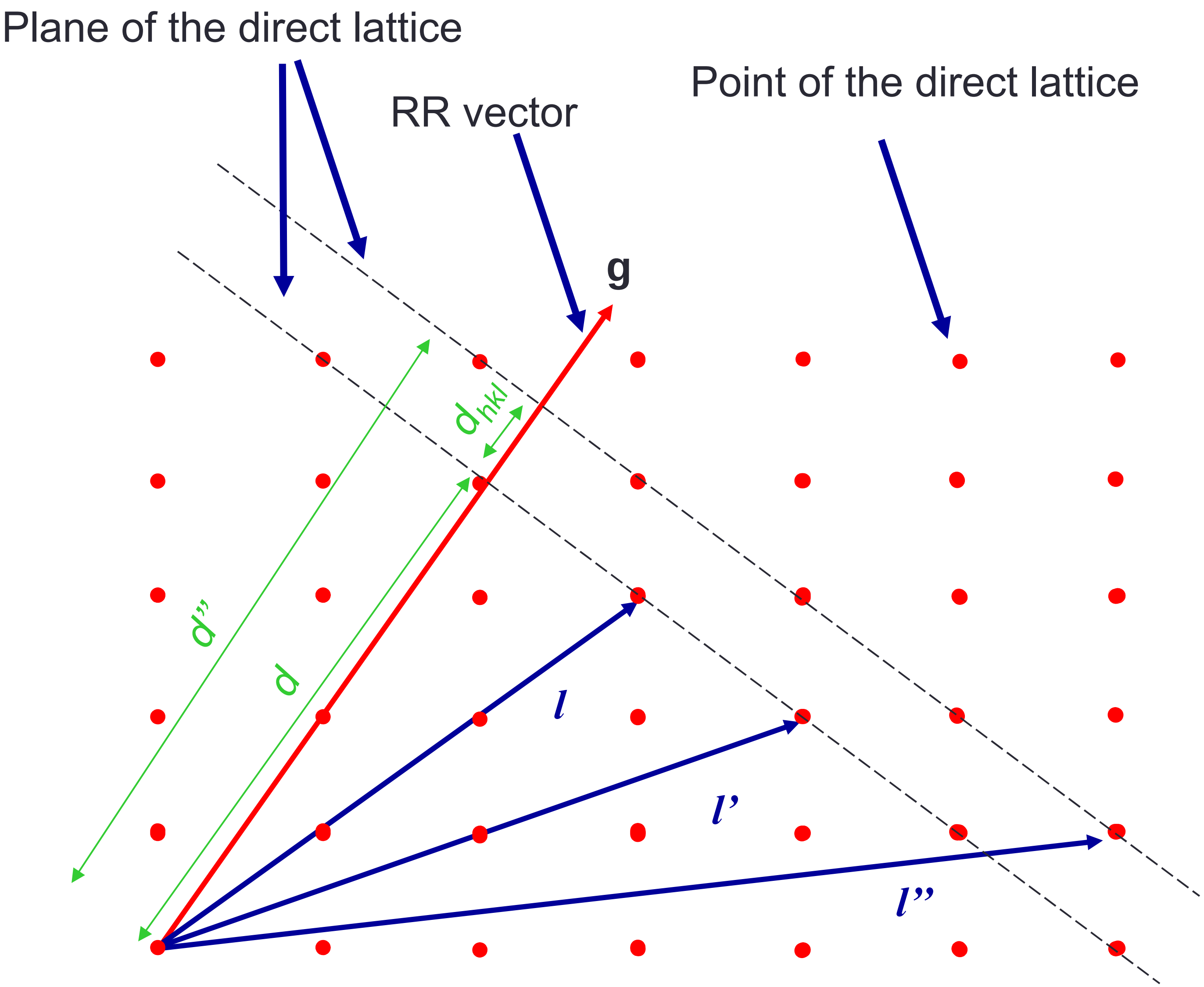
- We have (scalar product):

$$\overrightarrow{ON}.\overrightarrow{OP} = 2\pi\left[\underbrace{hn + kp + lq}_{\text{integer}}\right]$$

$$|g| = |ON| = \frac{2\pi}{|OP|}\left[hn + kp + lq\right]$$

Of course, unit of reciprocal lattice is :

$$\left[\vec{b}\right] = \frac{1}{length} = m^{-1}$$



Plane of the direct lattice

RR vector

Point of the direct lattice

Properties of the reciproqual lattice

- **Each vector of the reciprocal lattice is normal to a set of lattice planes of the direct lattice**

$$\vec{g} = g_1\vec{b}_1 + g_2\vec{b}_2 + g_3\vec{b}_3$$

$$\vec{l} = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$$

$$\vec{g}.\vec{l} = 2\pi(g_1l_1 + g_2l_2 + g_3l_3) = 2\pi N$$

- and $\vec{g}.\vec{l}$ represents the projection of the vector ***l*** on the direction of ***g***, which has the length « ? » .
- But there are infinitely many points of the lattice with this property (for example $l'_1 = l_1 - m x g_3$, $l'_2 = l_2 - m x g_3$, $l'_1 = l_1 + m x (g_2 + g_1)$)

$$\vec{g}.\vec{l}' = 2\pi(g_1l_1 + g_2l_2 + g_3l_3) = 2\pi N$$

- We have construct one of the lattice planes

Properties of the reciproqual lattice

- If the components of g have no common factor, then |g| is inversely proportionnal to the spacing of the lattice planes normal to ***g***.
  - if (g_1,g_2,g_3) have no common factors, then we can always find a lattice vector ***l''*** with components such that

$$\vec{g}.\vec{l''} = 2\pi(N+1)$$

- So d'' can be written:

$$d'' = \frac{2\pi(N+1)}{|g|} = \frac{2\pi N}{|g|} + \frac{2\pi}{|g|} = d + d_{hkl}$$

$$\boxed{d_{hkl} = \frac{2\pi}{|g|}}$$

- From these two geometrical results, we see that the simplest way of characterizing the planes of a lattice is by their normals, expressed as vectors of the reciprocal.

Properties of the reciproqual lattice

- Choose a plane with its normal ***g*** (a vector of reciprocal lattice)

$$\vec{g} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

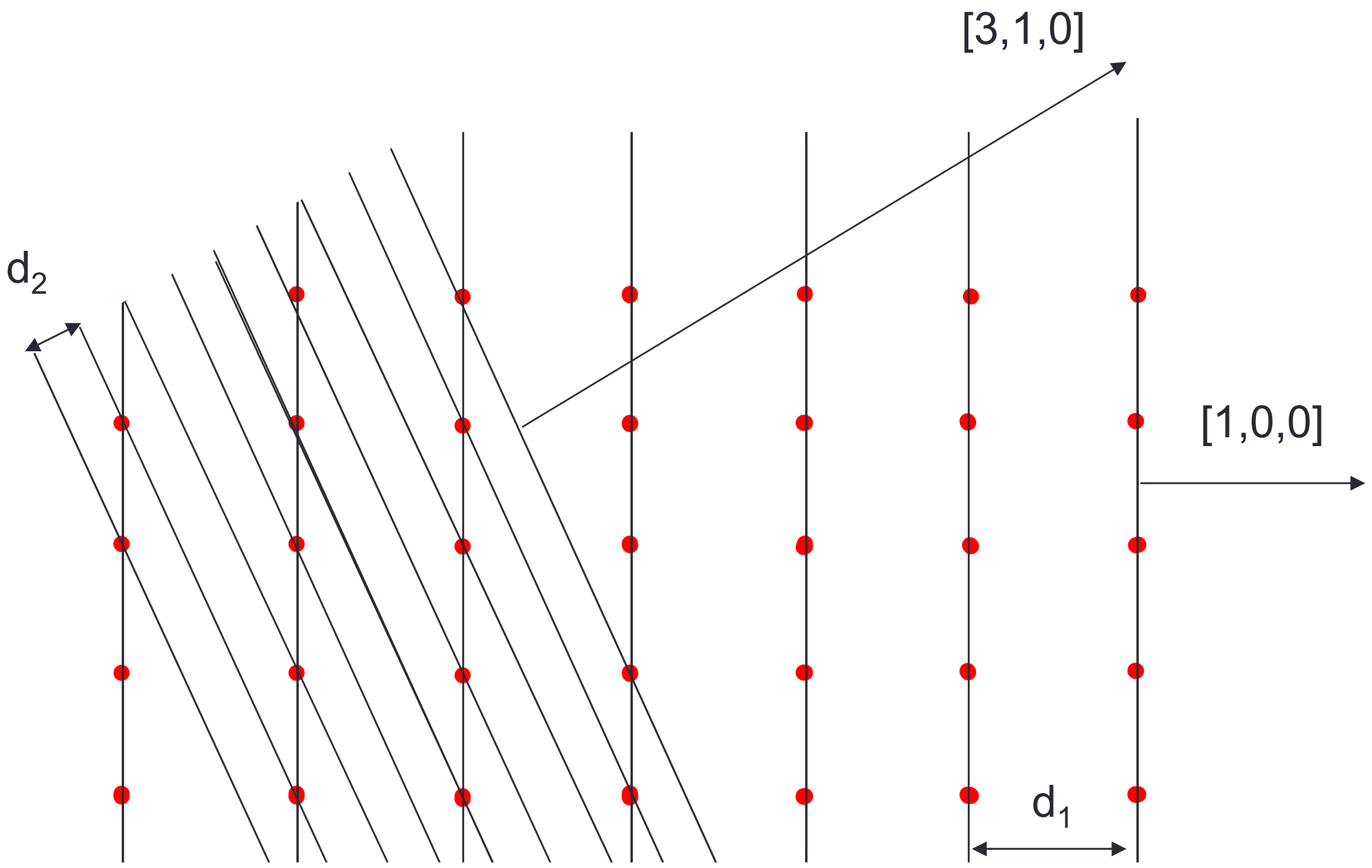
We get $\vec{g}.\vec{l} = 2\pi\left[hn + kp + lq\right] = 2\pi N$; verified for all points belong to this plane. If we choose a point with p=q=0, we get n=N/h, so, the choosen plane cut axis ***a*₁** at $d_1 = \frac{N}{h}a_1$. Same relation with d_2 and d_3.

$$d_1 = \frac{N}{h}a_1, d_2 = \frac{N}{k}a_2, d_3 = \frac{N}{l}a_3 \qquad d'_1 = \frac{N}{h}, d'_2 = \frac{N}{k}, d'_3 = \frac{N}{l}$$

En unité des vecteurs de base

$$\text{Example}: d'_1 = \frac{2}{3}, d'_2 = \frac{2}{4}, d'_3 = \frac{2}{5} \Longrightarrow \left(\frac{3}{2}, \frac{4}{2}, \frac{5}{2}\right) \Longrightarrow (3{,}4{,}5) = (h, k, l)$$

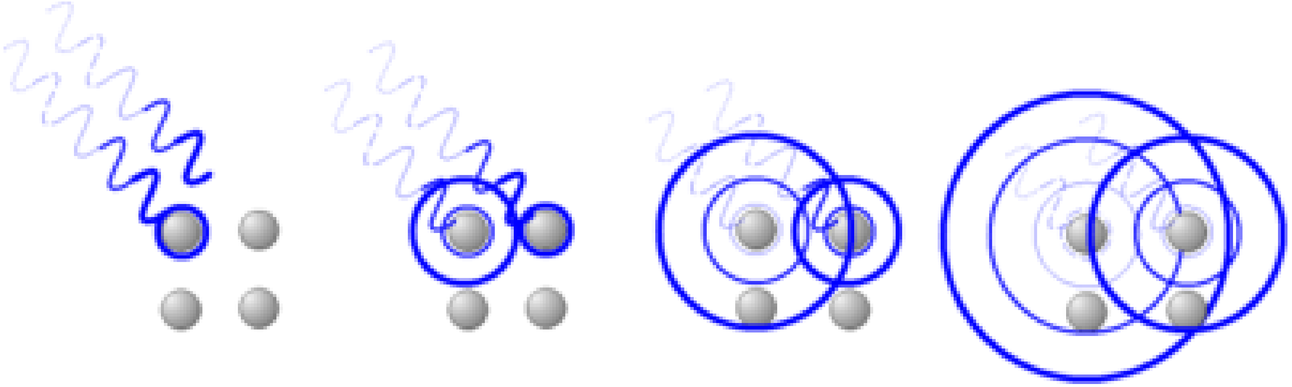
We obtain the same indexes for g (normal to the plane) and for the plane !


[3,1,0]
d$_2$
[1,0,0]
d$_1$

Physical meaning of planes – importance of reciprocal lattice

- Consider a crystal traversed by a wave :
  - EM (RX, Rγ)
  - Acoustic (phonons)
  - Particle wave (electrons, neutrons)

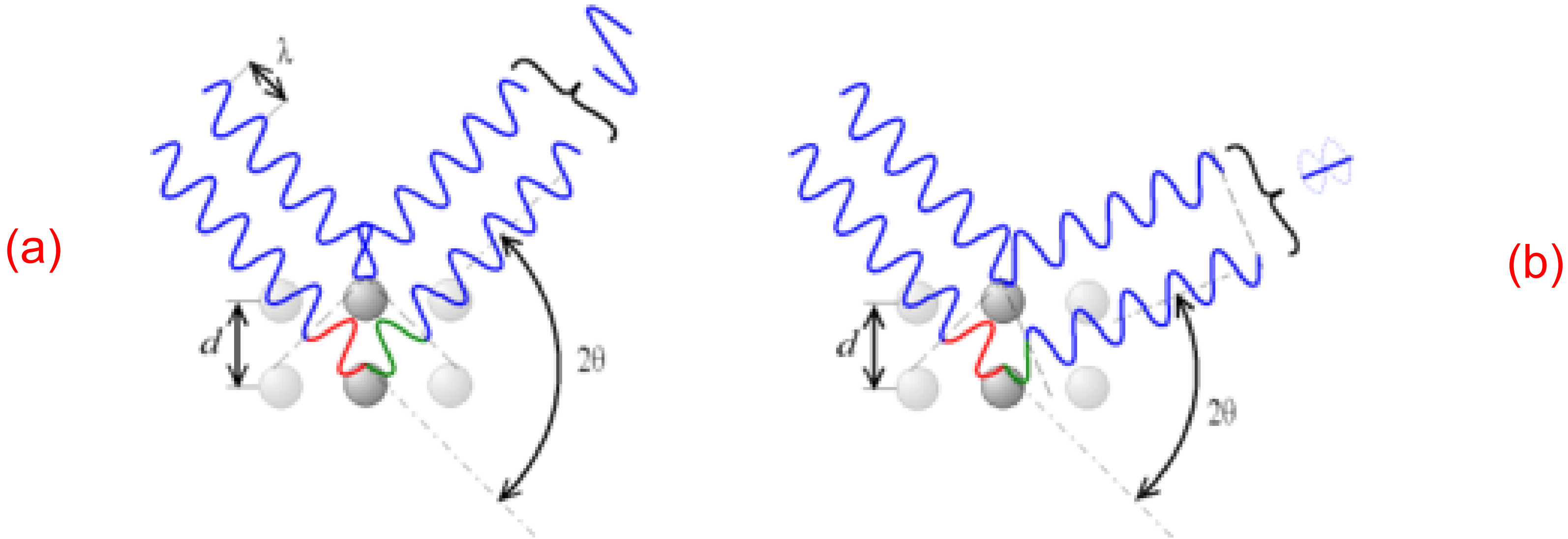
Electrons (electrons cloud) move and radiate in all directions. This is the diffusion effect (Rayleigh scattering)



Physical meaning of planes – importance of reciprocal lattice

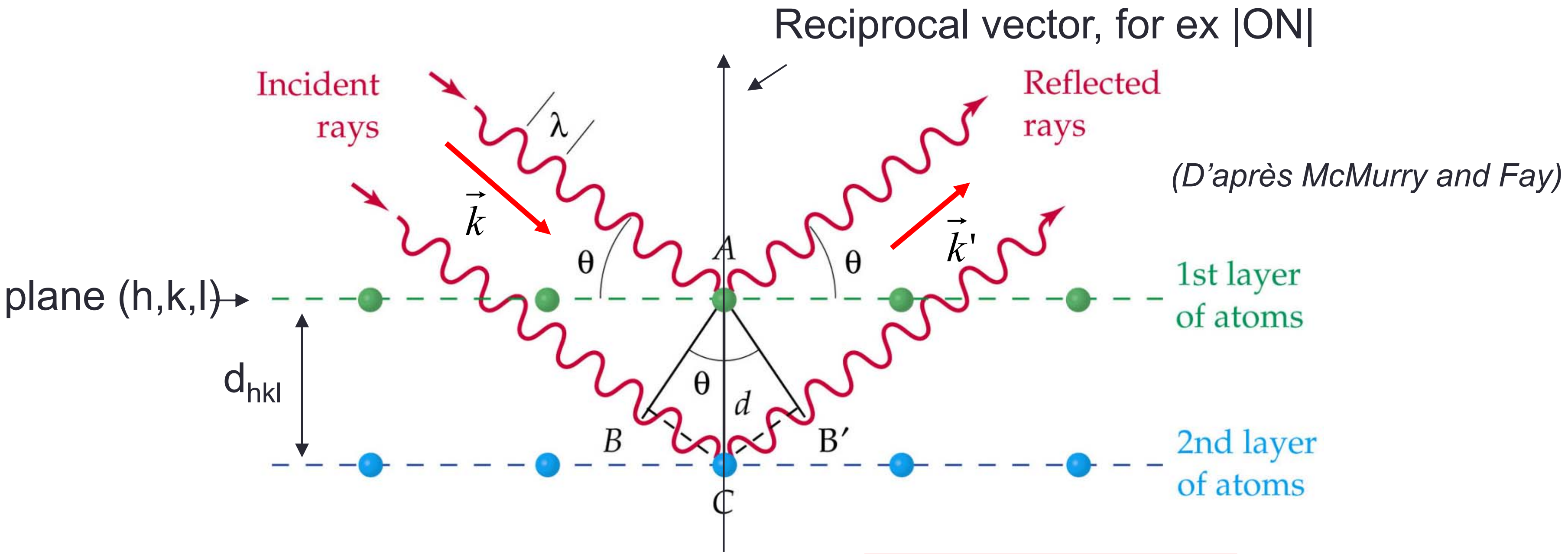
- Interferences between diffusing waves:
  - destrutively ⇔ no propagation (b)
  - Constructively ⇔ we can detect (« see ») them(a)

⇨ Bragg's diffraction condition



Physical meaning of planes – importance of reciprocal lattice

- ***Bragg law determination*** : elementary method.
  - Crystalline planes behave as mirrors
  - We calculate de path difference (ddm) between the two beams
  - Constructively interference ⇔ ddm = nλ



Reciprocal vector, for ex |ON|

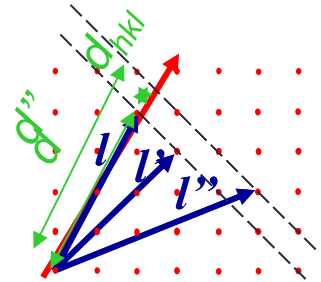
plane (h,k,l)

d_{hkl}

(D'après McMurry and Fay)

$$ddm = 2d_{hkl}\sin\theta \quad \Leftrightarrow \quad \boxed{2d_{hkl}\sin\theta = n\lambda}$$

Physical meaning of planes – importance of reciprocal lattice



- ***Bragg's law***: condition on vector of reciprocal lattice

$$\boxed{2d_{hkl}\sin\theta = n\lambda}$$

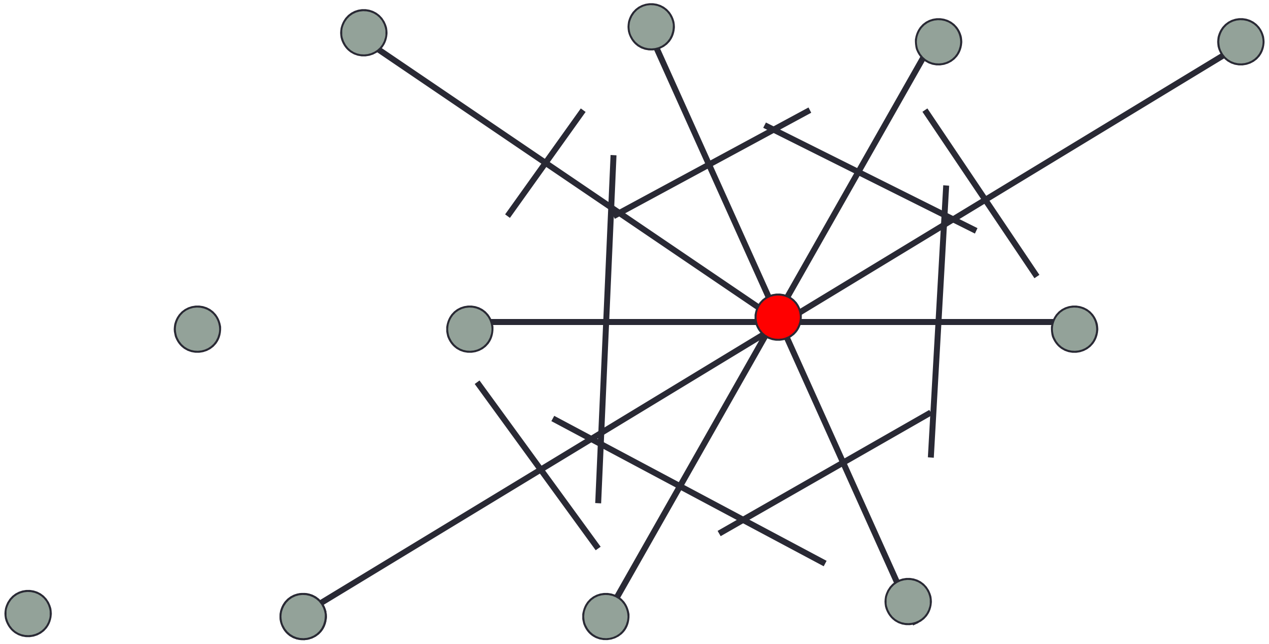
$$d_{hkl}.\left|\overrightarrow{ON}\right| = 2\pi \quad \Leftrightarrow \quad d_{hkl} = \frac{2\pi}{\left|\overrightarrow{ON}\right|} \quad \text{with } \overrightarrow{ON} \text{ vector of RL}$$

$$2.\frac{2\pi}{\left|\overrightarrow{ON}\right|}\frac{\sin\theta}{\lambda} = n \qquad \text{and wave vector } \left|\vec{k}\right| = \frac{2\pi}{\lambda}, \vec{1} = \frac{\overrightarrow{ON}}{\overline{\overline{ON}}}, \vec{k}.\vec{1} = \frac{2\pi}{\lambda}\sin\theta$$

$$2.\frac{\vec{k}.\vec{1}}{\left|\overrightarrow{ON}\right|} = 2\frac{\vec{k}}{\overline{\overline{ON}}}\frac{\overrightarrow{ON}}{\overline{\overline{ON}}} = 2\frac{\vec{k}}{\overrightarrow{ON}}\frac{\overrightarrow{ON}}{\overrightarrow{ON}} = n$$

$$2\bar{k} = n\,\overline{ON}, \quad \text{or} \quad \boxed{\bar{k} = n\frac{\overline{ON}}{2}}$$

Unity cell / Wigner-Seitz cell: first Brillouin zone



CHAPTER 2

Wave diffraction from a crystal

Reciprocal lattice

Brillouin zone

Introduction:

- The diffraction of waves ($k = 2\pi/\lambda$) by a crystal is present in two domains :
  - Cristallography:
    - X Rays difraction:

$$\boxed{E = h\nu = \frac{hc}{\lambda}} \qquad \boxed{\lambda = \frac{hc}{E} = \frac{12{,}4}{E(keV)}\ \mathring{A}}$$

- Neutrons diffraction
- Electrons diffraction

$\Big\}$ Wave – particle duality (de Broglie)

$$\boxed{\lambda_{deBroglie} = \frac{h}{p}} \boxed{E = \frac{p^2}{2m_{n/e}} = \frac{h^2}{2\lambda^2 m_{n/e}}} \boxed{\lambda_e(\mathring{A}) = \frac{h}{\sqrt{2m_e}\sqrt{E}} = \frac{12}{\sqrt{E(eV)}}}$$

Generality:

- The objective of crystallography: studying the directions in which the diffracted energy is maximum and deduce the distance between the lattice planes, the # of atoms of each of lattice planes, all this by measuring the scattered intensity

Generality:

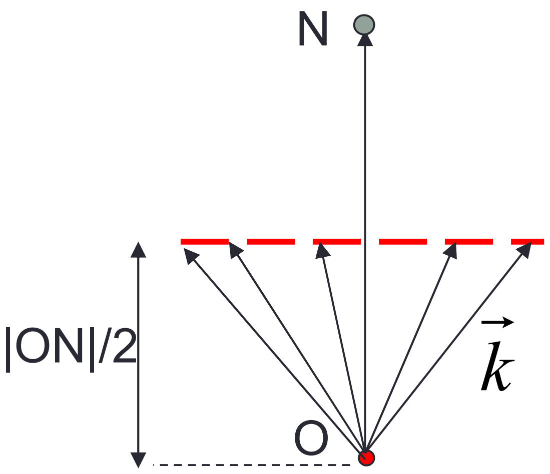
- The second field of interest :
  - Solid state physics: on utilise la condition de Bragg (maximum d’intensité diffractée) pour déterminer les λ électroniques qui ne peuvent se propager dans le cristal (elles sont diffractées!). On associe à chacune des ces λ satisfaisant à la loi de Bragg une bande d’énergie pour l’électron qu’on appelle bande interdite (« gap »). We use the Bragg condition (maximum diffracted intensity) to determine the electronic wave length λ that can not propagate in the crystal (they are diffracted!). Is associated with each of those λ satisfying the Bragg's law an energy band for the electron, called band gap (or "gap").

Bragg's law

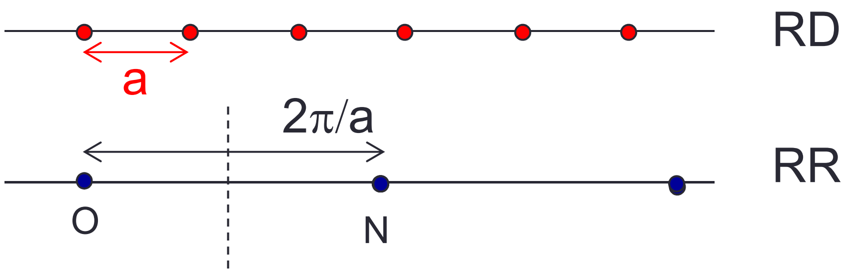
- Elementary method (see previous chapter)

$$\boxed{2d_{hkl}\sin\theta = n\lambda}$$

$$2\overline{k} = n\,\overline{ON}, \quad \text{or} \quad \overline{k} = \boxed{n\,\frac{\overline{ON}}{2}}$$



Example 1: 1D net

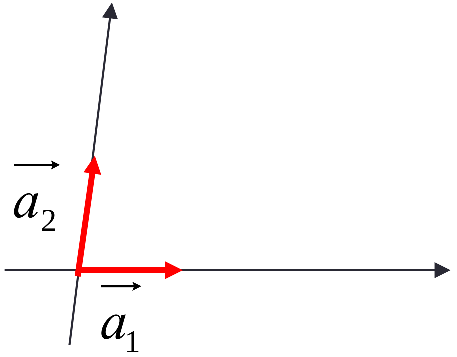


• if –π/a < *k* < π/a, wave is not diffracted. This is the first Brillouin zone

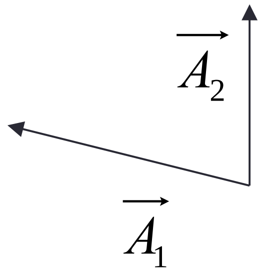
• if k = ± π/a, wave is diffracted, ⇔ *k* is in the limit of the first Brillouin zone

Bragg's law / Brillouin zone

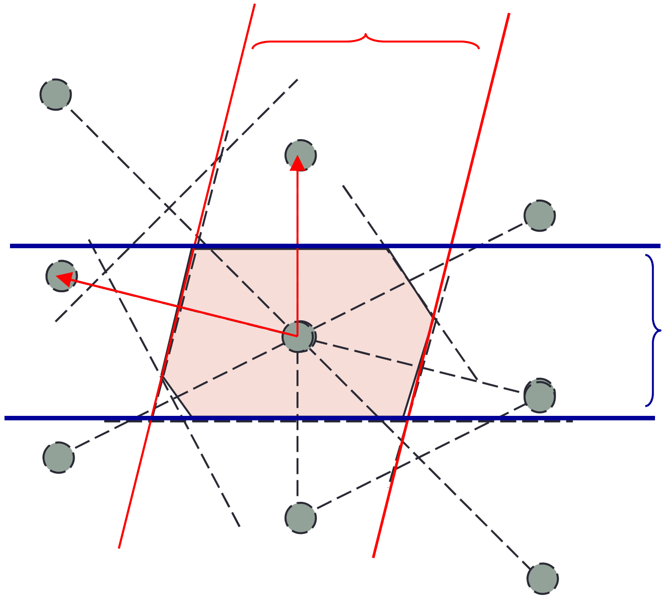
- Example 2: 2D lattice



Direct lattice



Reciprocal latticeR

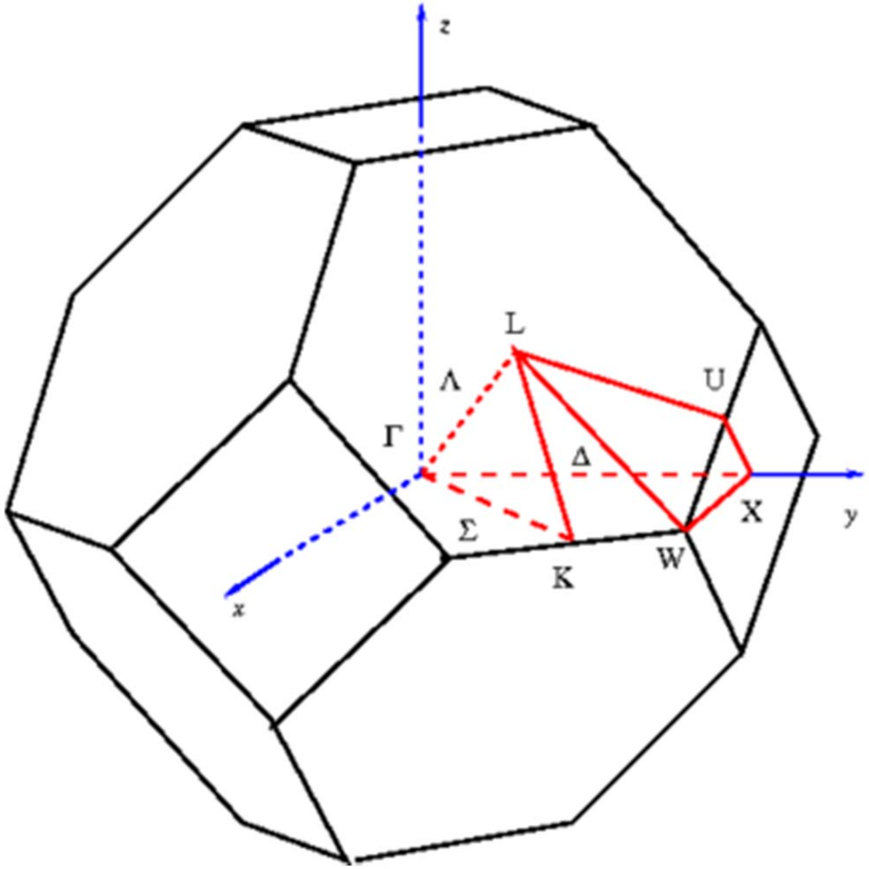


1° ZB ⊥ A_1 (// a_2)

1° ZB ⊥ A_2 (// a_1)

Waves with wavevector inside the Brillouin zone can propagate in the crystal.

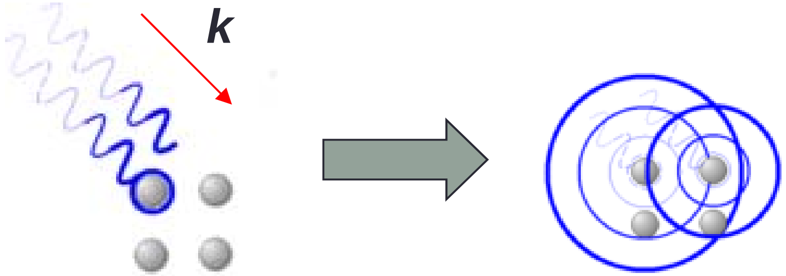
Brillouin Zone of FCC crystal



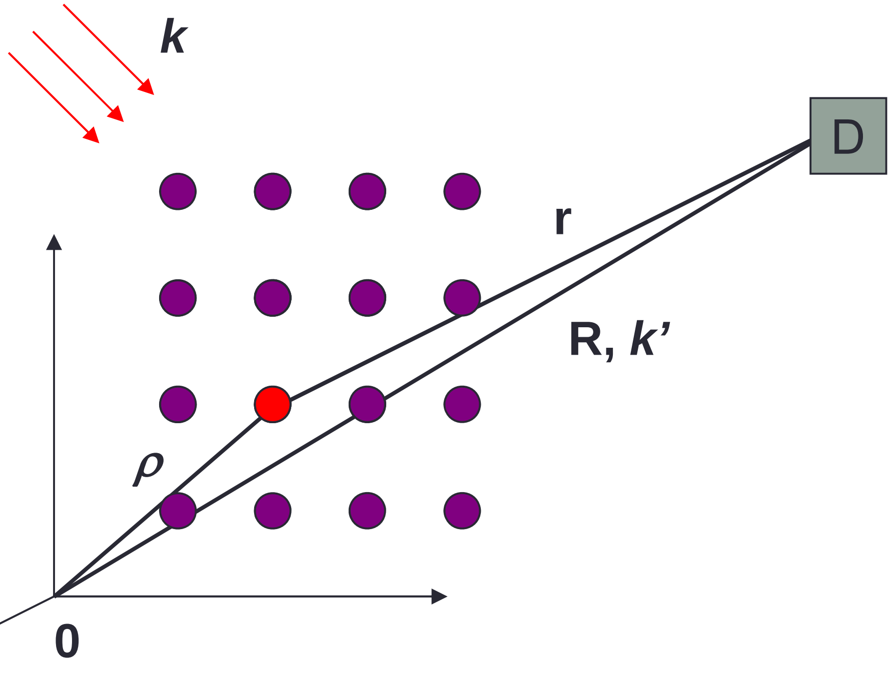
http://en.wikipedia.org/wiki/Brillouin_zone

Bragg law: Laue equations

- <u>Direct method</u>: using scattering theory for optical waves



scattering : incident waves send off spherical wave



- ***k, k'*** : incident/diffused wave vector
- ρ: scattering atom position
- **r** : atom/detector distance
- **R**: position of a detector(far from crystal)

Bragg law: Laue equations

- Consider a plane wave at the position $\vec{\rho}$ described by the field :

$$\boxed{F(\vec{\rho}) = F_0 \exp i(\vec{k}.\vec{\rho} - \omega t)}$$

- Wave with a wave vector $\vec{k}$, angular frequency ω and wave length $\lambda = \frac{2\pi}{k}$
- We put the crystal into the beam. Origin O is arbitrarily chosen
- Hypothesis: incident beam is not affected by the crystal
  - It means no energy loss

Bragg law: Laue equations

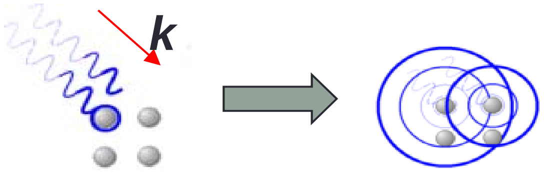
- Field of incident beam at ρ is given by :

$$\boxed{F(\vec{\rho}) = F_0 e^{i\vec{k}.\vec{\rho}} e^{-i\omega t}} \qquad \text{(3D)}$$

- at $\vec{\rho}$, we have an intercation between atoms and incident wave: we get a scattered spherical wave . The scatterd field at point $\vec{r}$ (the detector) is given by:

$$\boxed{F_{sc}(\vec{r}) = fF_0 \frac{e^{i\vec{k}\vec{\rho}} e^{i(\vec{k}\vec{r}-\omega t)}}{r}}$$

Scattering factor: fraction of incident wave scattered by an atom



scattering : creation of a spherical wave

- The detector position is far compared to the size of the crytal

$$r \approx R - \rho\cos(\boldsymbol{\rho},\mathbf{R}) \approx R$$

Bragg law: Laue equations

- Scaterred wave:

$$\boxed{F_{sc}(\vec{r}) = fF_0 \frac{e^{i\vec{k}\vec{\rho}} e^{i(\vec{k}\vec{r}-\omega t)}}{r}}$$

$$r \approx R - \rho\cos(\boldsymbol{\rho},\mathbf{R}) \approx R$$

$$\boxed{F_{sc}(\vec{r}) = \frac{fF_0 e^{-i\omega t} e^{i\vec{k}.\vec{\rho}+i\vec{k}\vec{R}-ik\rho\cos(\vec{\rho},\vec{R})}}{R} = F_{sc}(\vec{R})}$$

Bragg law: Laue equations

- We writte $i\vec{k}.\vec{\rho} - ik\rho\,\mathbf{cos}(\vec{\rho},\vec{R})$ differently:

$$\boxed{ik\rho\cos(\vec{\rho},\vec{R}) = ik\rho\cos(\vec{\rho},\vec{k}') = ik'\rho\cos(\vec{\rho},\vec{k}') = i\vec{k}'.\vec{\rho}}$$

- $\vec{k}'$ is the scattered wave vector along the direction $\vec{R}$, with the same norm than $\vec{k}$ (elastic scattering)

- Scattering relation becomes:

$$\boxed{F(\vec{R}) = \frac{fF_0 e^{-i\omega t} e^{i\vec{k}.\vec{\rho} + i\vec{k}\vec{R} - ik\rho\cos(\vec{\rho},\vec{R})}}{R}} \quad \boxed{F(\vec{R}) = \frac{fF_0 e^{-i\omega t} e^{i\vec{k}\vec{R}}}{R} e^{-i\overrightarrow{\Delta k}.\vec{\rho}}} \quad \boxed{\overrightarrow{\Delta k} = \vec{k}' - \vec{k}}$$

- We now sum the signal from all the atoms on the lattice sites:

$$\boxed{\begin{aligned} F(\vec{R}) &= \sum_p \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R}\left[e^{-i\overrightarrow{\Delta k}.\vec{\rho}_p} f_p\right] \\ F(\vec{R}) &= \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p f_p \left[e^{-i\overrightarrow{\Delta k}.\vec{\rho}_p}\right] \end{aligned}}$$

Bragg law: Laue equations

- Can the amplitude of the filed be zero?

$$\boxed{F(\vec{R}) = \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p f_p \left[e^{-i\overrightarrow{\Delta k}.\vec{\rho}_p} \right] = 0\,?}$$

- For a large number of sites (identical atoms) and this is the case, the sum is zero if : $\boxed{\rho_p.\Delta k = 2\pi n}$

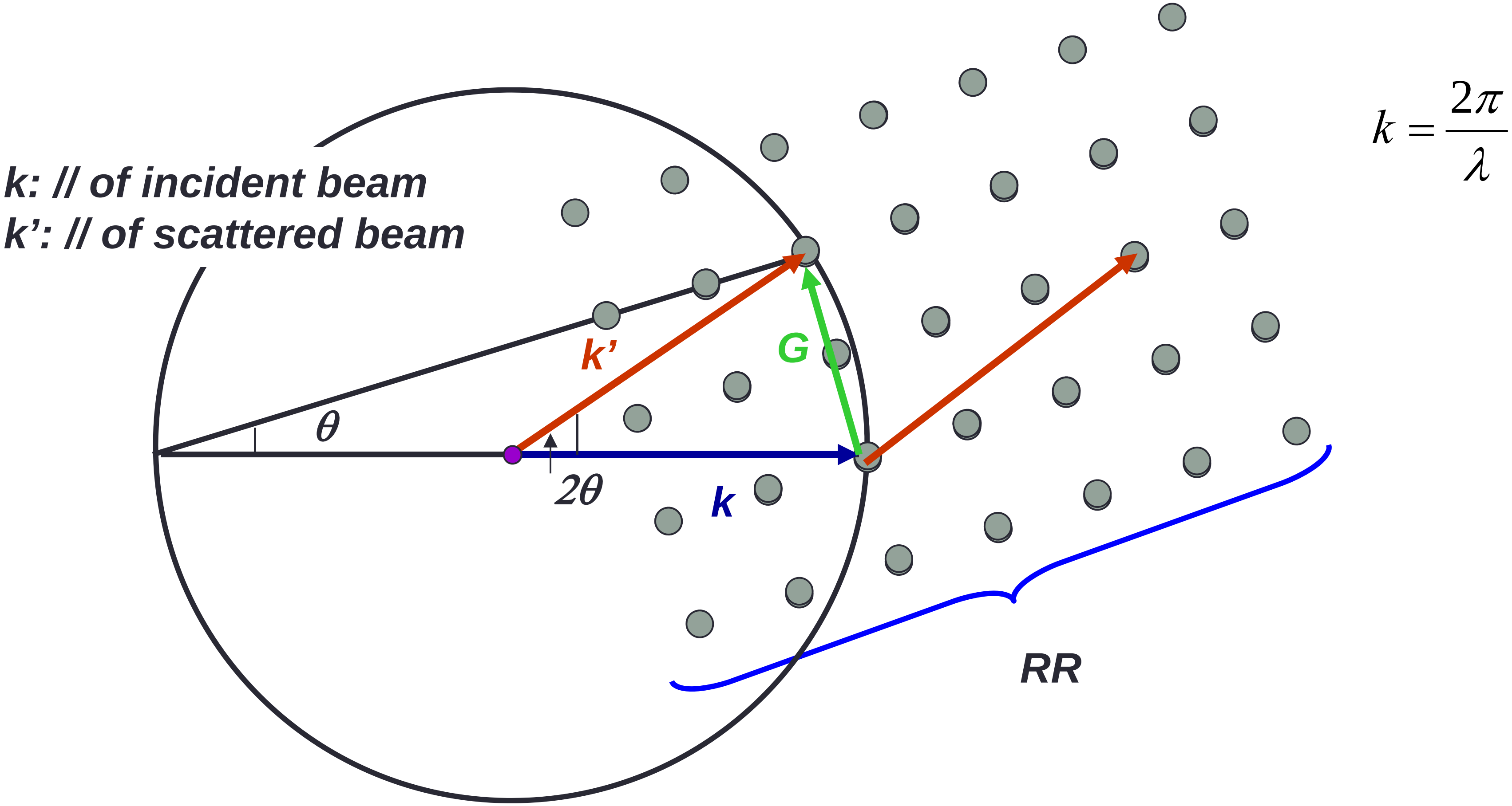
- However, this is the definition of a reciprocal lattice vector. thus Δ**k** (ou scattering vector) has to be a reciprocal lattice vector **G**, for non zero scattered intensity.

Bragg law: Laue equations

- Conclusion: *the condition of a high diffraction intensity is satisfied only when the wave vector is scattered by a reciprocal lattice vector*

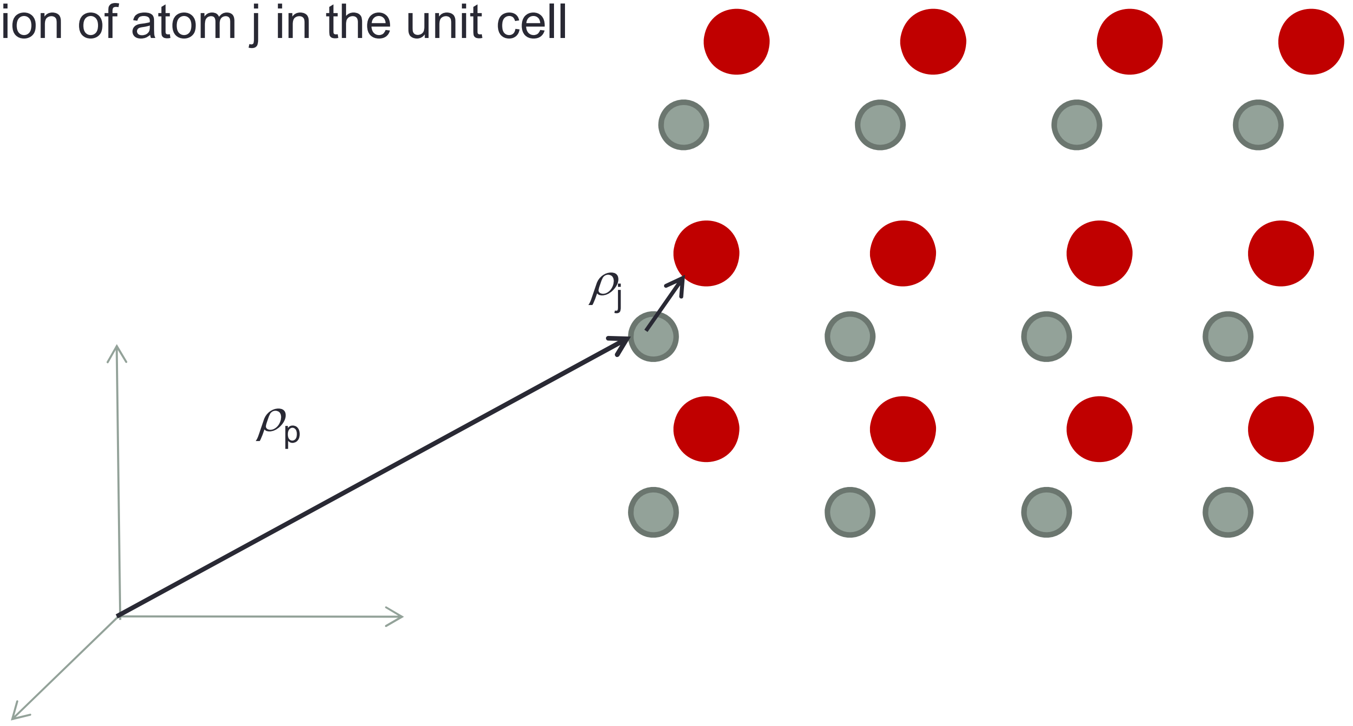
Laue equations (Ewald sphere)

- Elastic scattering of photons (no enery loss) ⇔|***k***| =|***k'***| .



$$k = \frac{2\pi}{\lambda}$$

- So far we have considered that scattering factor f_p is the same for all the sites and that there is only one atom per basis. This is not true, specially for semiconductors. We will now generalize the conditions for diffraction peaks:
  - n for # atoms in the basis
  - ρ_p for the position of unity cell
  - ρ_j for the position of atom j in the unit cell



Bragg law: Laue equations

- Scattering factor

$$\boxed{F(\vec{R}) = \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p f_p \left[e^{-i\Delta\vec{k}.\vec{\rho}_p} \right]} \Rightarrow \boxed{\frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p \sum_j f_j \exp\left[-i(\rho_p + \rho_j).\Delta k \right]}$$

  - We describe the scattering from each of the basis *j* atom by a factor f_j (depending of the nature of the atom)
  - The summation is separated into two summations – one over the lattice sites (4 in FCC !) and one over the atoms in the basis (2 in the diamond !)

$$\boxed{F(\vec{R}) = \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p \exp\left[-i\underset{\substack{\uparrow \\ \text{Structure description}}}{\rho_p}.\Delta k \right] \sum_j f_j \exp\left[-i\underset{\substack{\uparrow \\ \text{Basis description}}}{\rho_j}.\Delta k \right]}$$

$$F(\vec{R}) = \frac{F_0 e^{i\vec{k}\vec{R}} e^{-i\omega t}}{R} \sum_p \exp\left[-i\rho_p.\Delta k\right] \sum_j f_j \exp\left[-i\rho_j.\Delta k\right]$$

Structure description

Basis description

$$\overrightarrow{\rho_j}.\overrightarrow{\Delta k} = \overrightarrow{\rho_j}.\vec{G}$$

$$\overrightarrow{\rho_j} = x_j\vec{a} + y_j\vec{b} + z_j\vec{c} \quad \text{et} \quad \vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

$$\overrightarrow{\rho_j}.\vec{G} = (x_j\vec{a} + y_j\vec{b} + z_j\vec{c}).(h\vec{A} + k\vec{B} + l\vec{C})$$

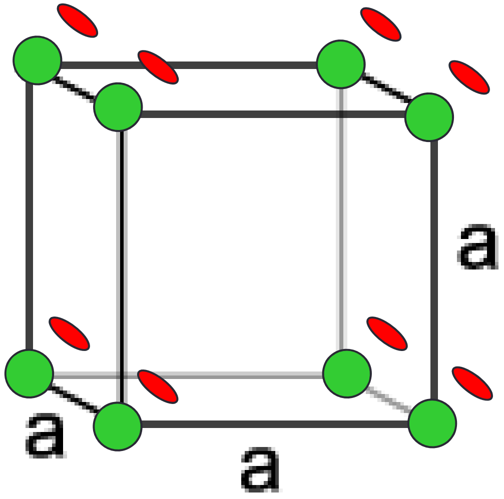
$$\overrightarrow{\rho_j}.\vec{G} = 2\pi(x_jh + y_jk + z_jl)$$

$$\overrightarrow{\rho_p}.\vec{G} = 2\pi(x_ph + y_pk + z_pl)$$

Structure factor and atomic form factor

- Atomic form factor: represents how the atom scatters the X-Rays impinging upon it. It depends essentially of electron cloud (Coulomb charge density), so the nature of the atom.

2 differents atoms in the basis



Each node have two diffrents atoms ⇔ we have to modify the relation

ρ_p : position of the p node in the lattice

ρ_j : position of the atom j in the basis (here 2 atoms in the base so two differents « j » atoms).

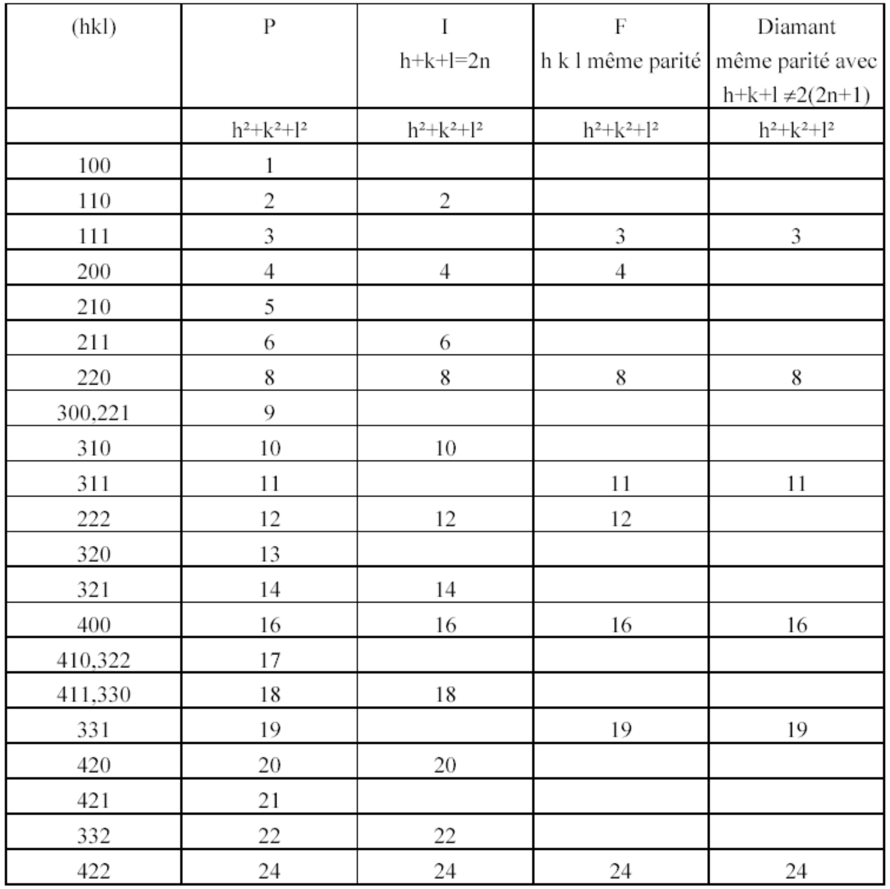
$$\boxed{S_{hkl} = \sum_j f_j \exp[-i2\pi(x_j h + y_j k + z_j l)] \sum_p \exp[-i2\pi(x_p h + y_p k + z_p l)]}$$

We take into account the degenerescence of the basis

Structure factor and atomic form factor

$$S_{hkl} = \sum_{j} f_j \exp[-i2\pi(x_j h + y_j k + z_j l)] \sum_{p} \exp[-i2\pi(x_p h + y_p k + z_p l)]$$

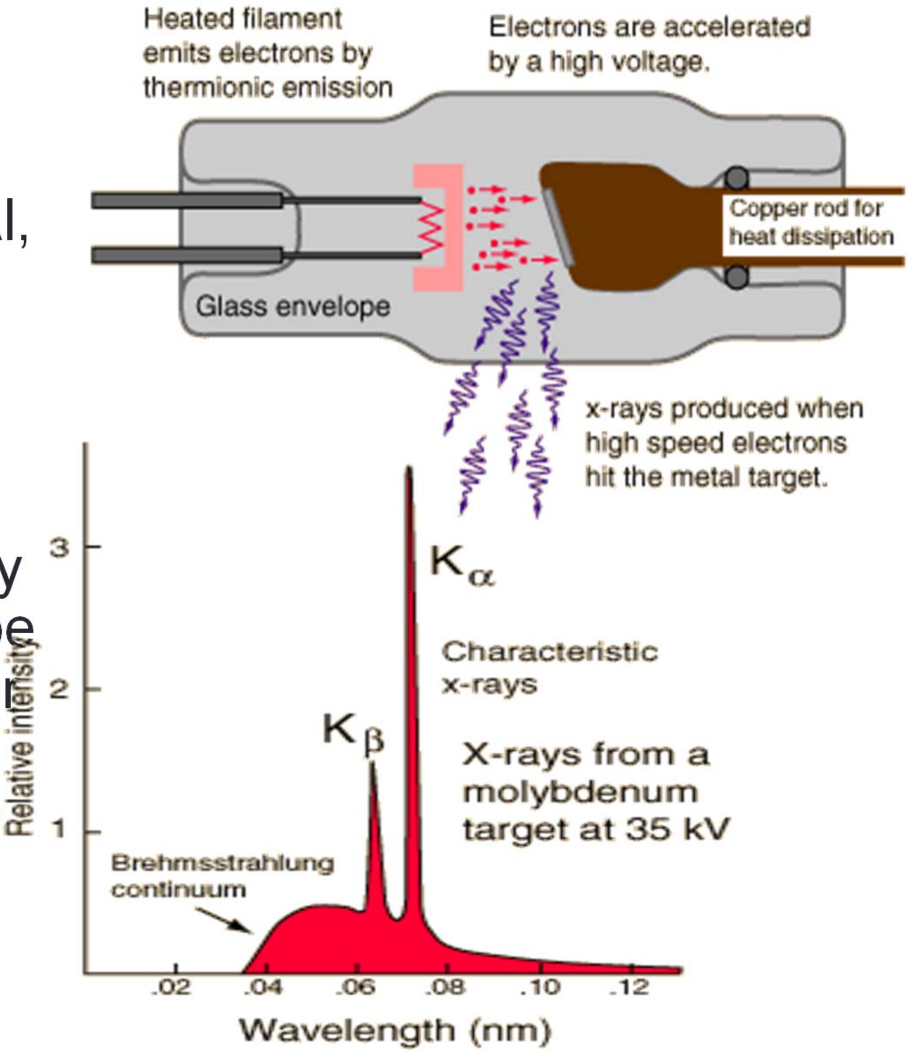
Altough the Bragg (Laue) condition is verified, the periodicity of the crystal conducts to supplementaries « zero conditions »(S_{hkl} = 0), more or less numerous, depending of the crystalline structure.



(hkl)	P	I h+k+l=2n	F h k l même parité	Diamant même parité avec h+k+l ≠2(2n+1)
	$h^2+k^2+l^2$	$h^2+k^2+l^2$	$h^2+k^2+l^2$	$h^2+k^2+l^2$
100	1			
110	2	2		
111	3		3	3
200	4	4	4	
210	5			
211	6	6		
220	8	8	8	8
300,221	9			
310	10	10		
311	11		11	11
222	12	12	12	
320	13			
321	14	14		
400	16	16	16	16
410,322	17			
411,330	18	18		
331	19		19	19
420	20	20		
421	21			
332	22	22		
422	24	24	24	24

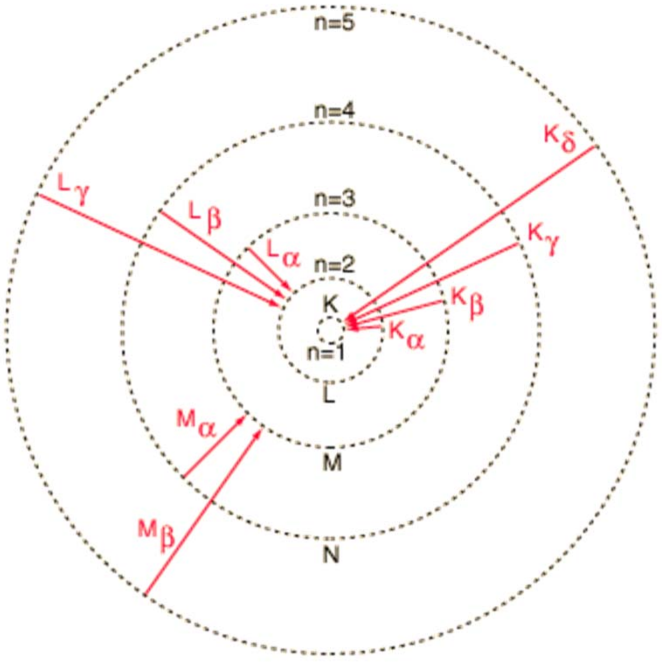
X-Rays and diffraction methods.

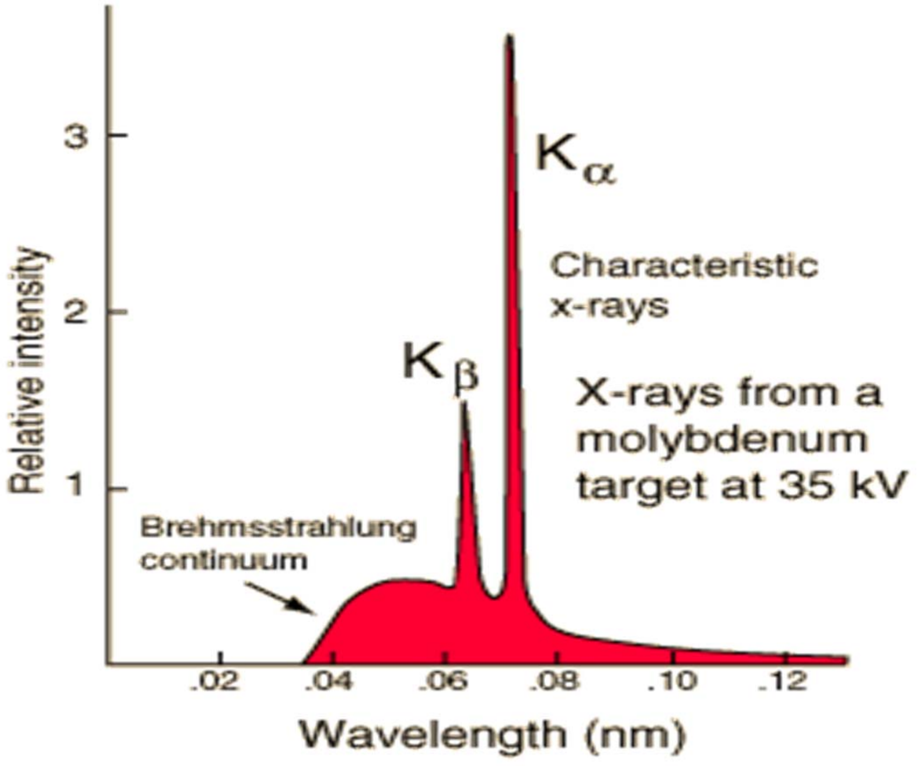
- X-Rays:
  - Electrons are accelerated
  - Electrons hit a target (Cu, Mo, Al, …)
  - 2 effects:
    - braking⇔ deceleration radiation (“brehmsstrahlung spectrum”)
    - Recycling of X-Rays produce by braking ⇔ core electrons can be excited ⇔ electrons from higher energy levels then fill up the vacancy and X-ray photons are emitted



X-Rays and diffraction methods.

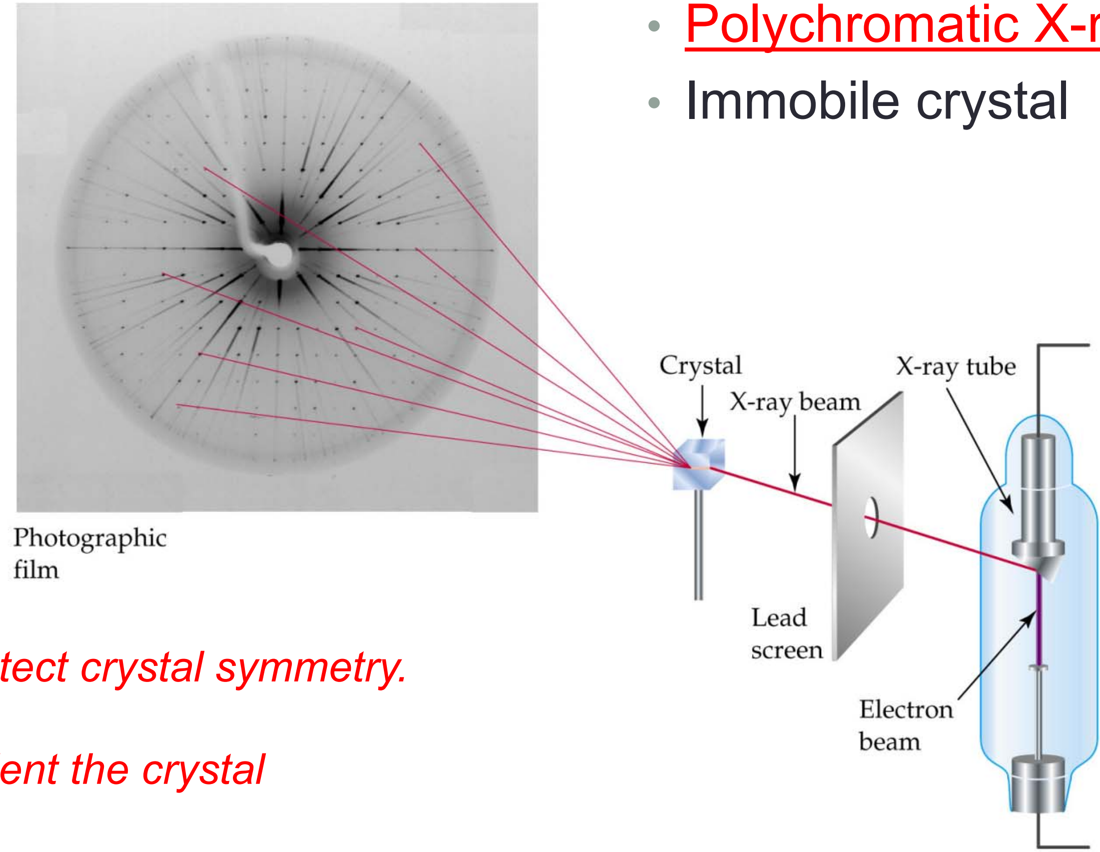
- X-Rays:
  - Discrete Spectrum : signature of the target (Cu, Mo, Al …)





Experimental methods for X-rays diffraction

- <u>Laue Method:</u>
  - monocrystal
  - <u>Polychromatic X-rays</u>
  - Immobile crystal

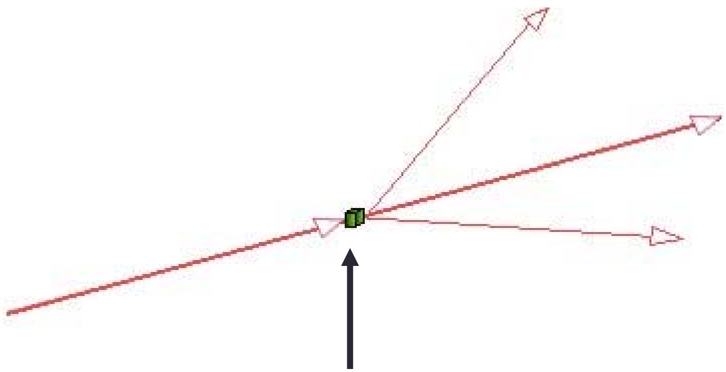


(D'après McMurry and Fay)

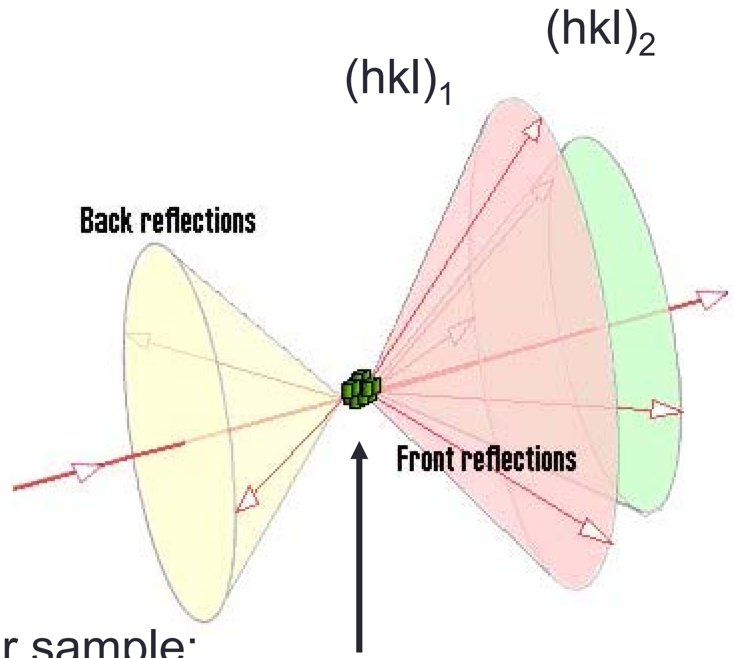
- *To detect crystal symmetry.*
- *To orient the crystal*

Experimental methods for X-rays diffraction

- Powder method:
  - monochromatic X-Rays



1 monocrystal ⇔ 1 plane (hkl) has the « right » angle of Bragg ⇔ 1 scattered beam

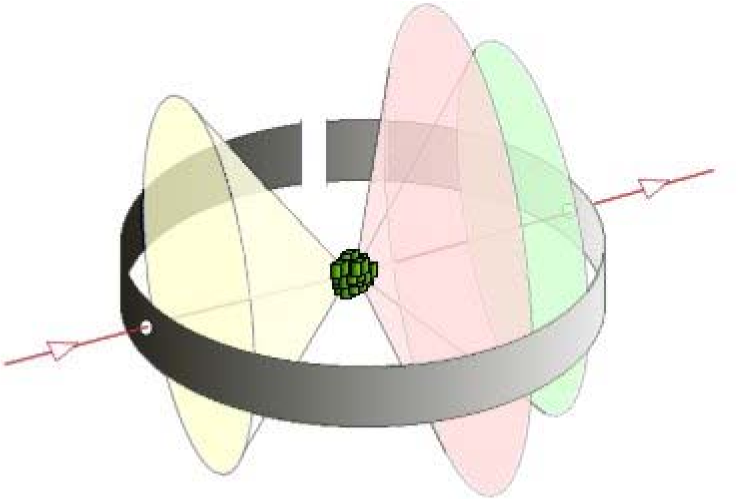


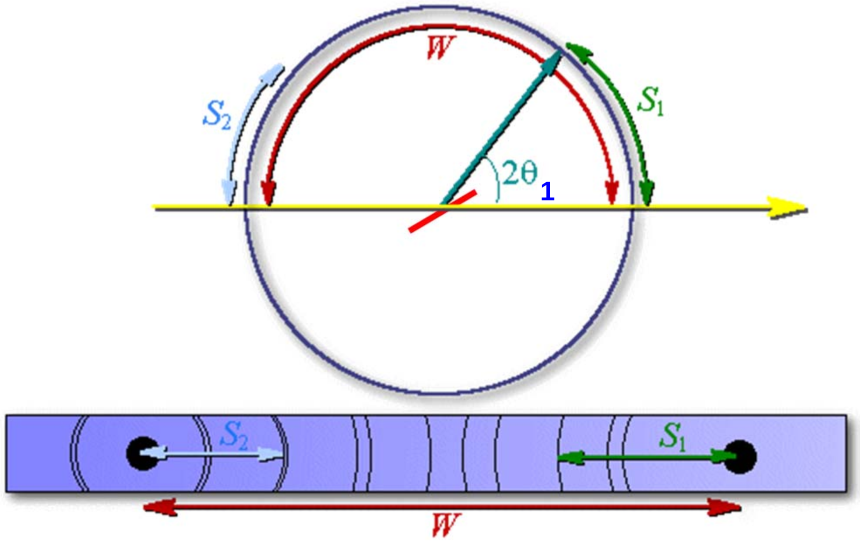
Powder sample:

Thousands of small „crystals“ (1 - 10 μm)
=> Statistical orientation of crystallites
=> Bragg‘s condition most likely valid for each lattice plane (in fact all the planes present in the crystal)
=> Constructive interference of diffracted beams

Experimental methods for X-rays diffraction

- Powder method:
  - R: radius of the Debye –Scherrer chamber
  - W=πR : half perimeter of the chamber



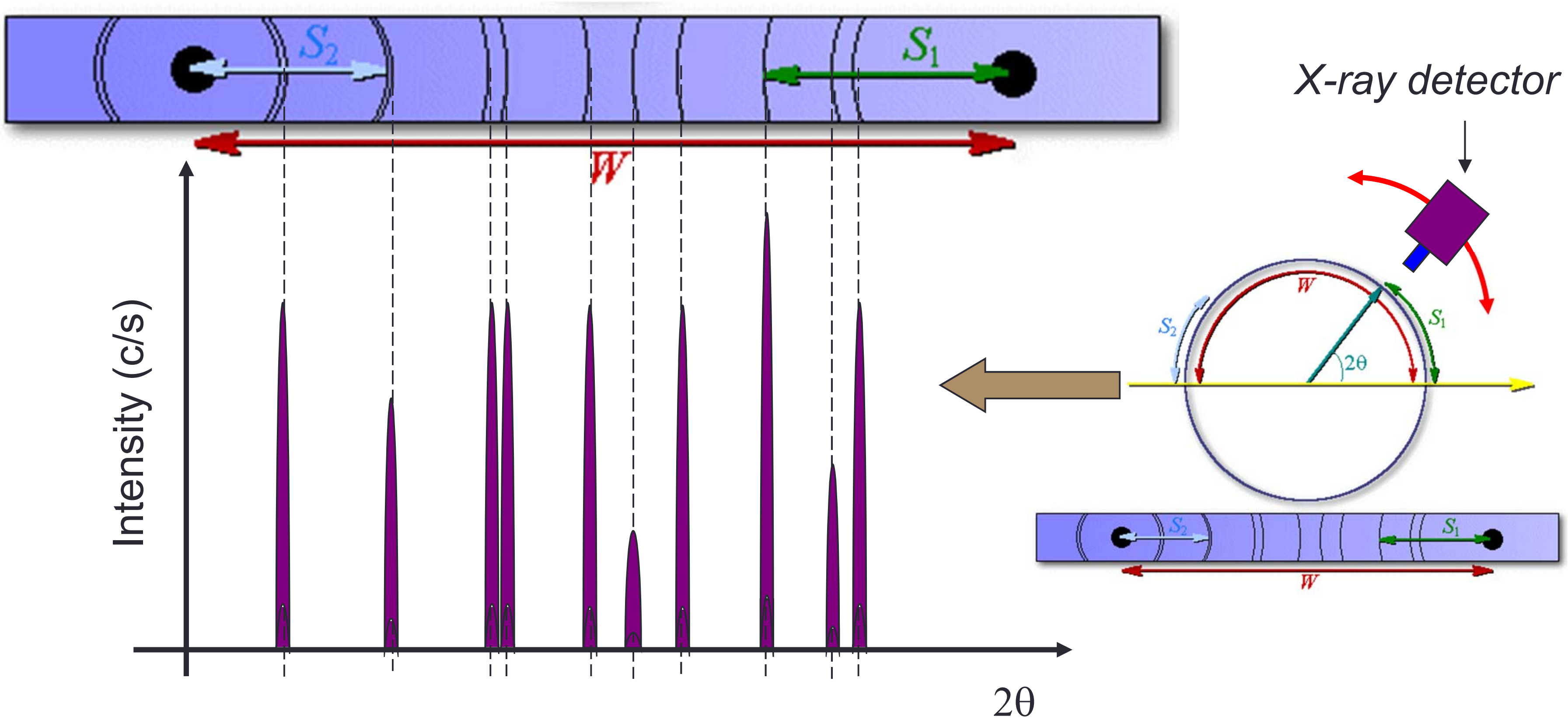


$$S_1 = 2R\theta_1$$

Measure S_1 allow to determine θ, the Bragg angle

Experimental methods for X-rays diffraction

- Powder method:



Experimental methods for X-rays diffraction

- Powder method:
  - Function of the structure, particular peaks are present or not ⇔ we can determine the crystalline structure.
  - Peak intensity is also an important parameter.
  - Allow to determine lattice parameter
  - It works also in mixed powder (mixed crystal)

CHAPITER 3

Wave mechanics :

Schrödinger equation

The end of the classical mechanics?

- *mater:*
  - Position
  - speed (momentum)

  - Newton law

Six variables can perfectly define the state of each particle

- *light:*
  - Electric field
  - Magnetic field

  - Maxwell relation

we can not transform the radiation into particles maintained localized in space ⇔ interference and diffraction process

The end of the classical mechanics?

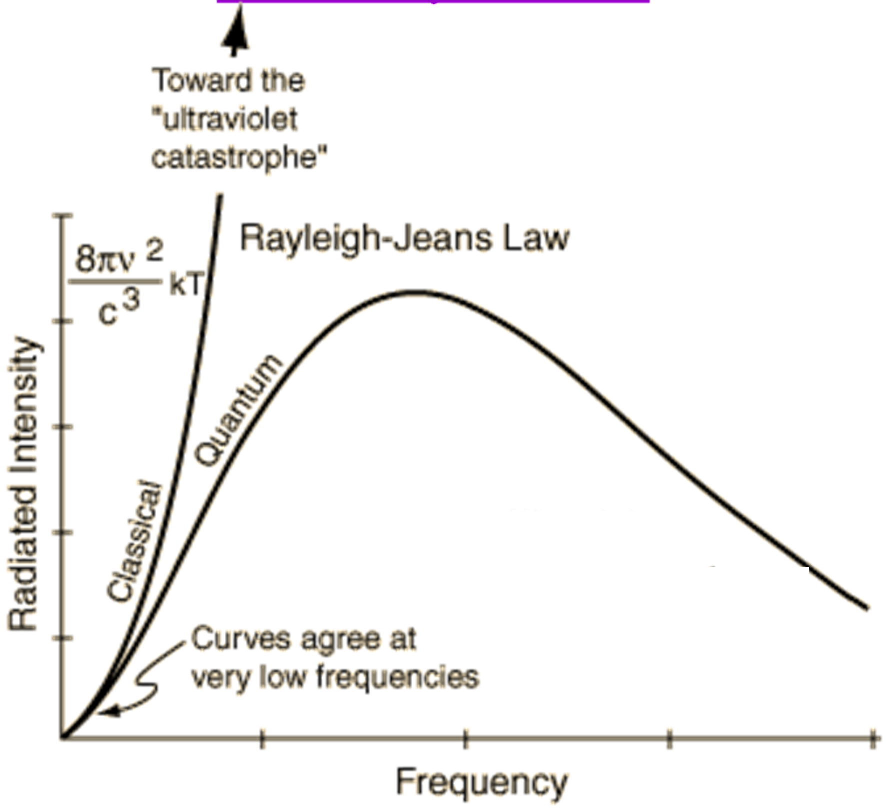
- *In the early 20th century :*
  - *Particle theory of the matter:*
    - « works » even at microscpics scale
    - But very complex at this scle ⇔ statistics mechancs

  - *Wave theory of ligth:*
    - Accepted since Fresnel work
    - All known phenomena of light are interpreted
    - Maxwell relation + radio waves (Hertz) ⇔ optical and electricity synthesis

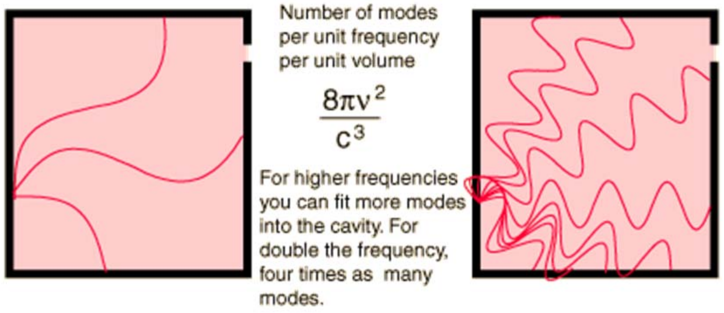
The end of the classical mechanics?

- New experiences / discoveries pose problems of interpretation:

Black body radiation



Black body: object which absorbs all impinging radiation



Number of modes per unit frequency per unit volume

$$\frac{8\pi\nu^2}{c^3}$$

For higher frequencies you can fit more modes into the cavity. For double the frequency, four times as many modes.

Inside the cavity, the electromagnetic field is equivalent to a set of independant harmonic oscillators. Their mean energy (assuming that the energy can vary continuously) is given by :

$$\overline{E} = \frac{\int_0^\infty E e^{-E/kT} dE}{\int_0^\infty e^{-E/kT} dE} = \mathrm{kT}$$

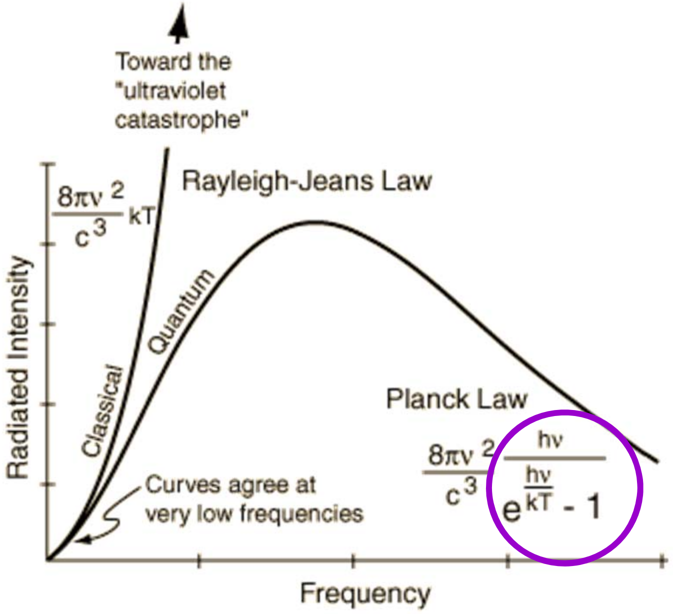
The end of the classical mechanics?

- New experiences / discoveries pose problems of interpretation:

Black body radiation

M. Planck : He postulates that the energy exchange between matter and radiation are not made continuously but by indivisible and discrete quantities: quanta of energy. He shows that the relationship between energy and frequency is given by:

$$E_n = n.h\nu$$



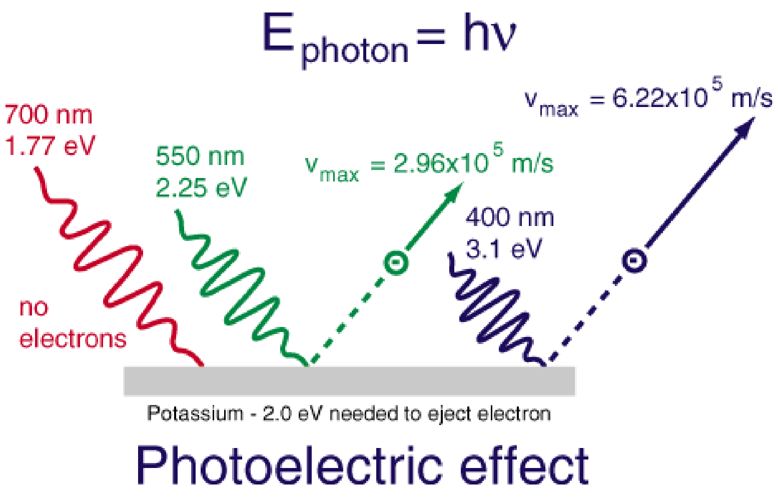
M. Planck : energy and frequency are dependent ⇔ allowed modes are more and more difficult to populate. In the cavity, (the black body), atoms in the wall act as oscillators with a frequency ν and the atom's energy is given by:

$E_n = n.h\nu$

$$\overline{E} = \frac{\sum_{n=1}^{\infty} E_n e^{-E/kT}}{\sum_{n=1}^{\infty} e^{-E/kT}} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

The end of the classical mechanics?

- New experiences / discoveries pose problems of interpretation:
  - photo électric effect

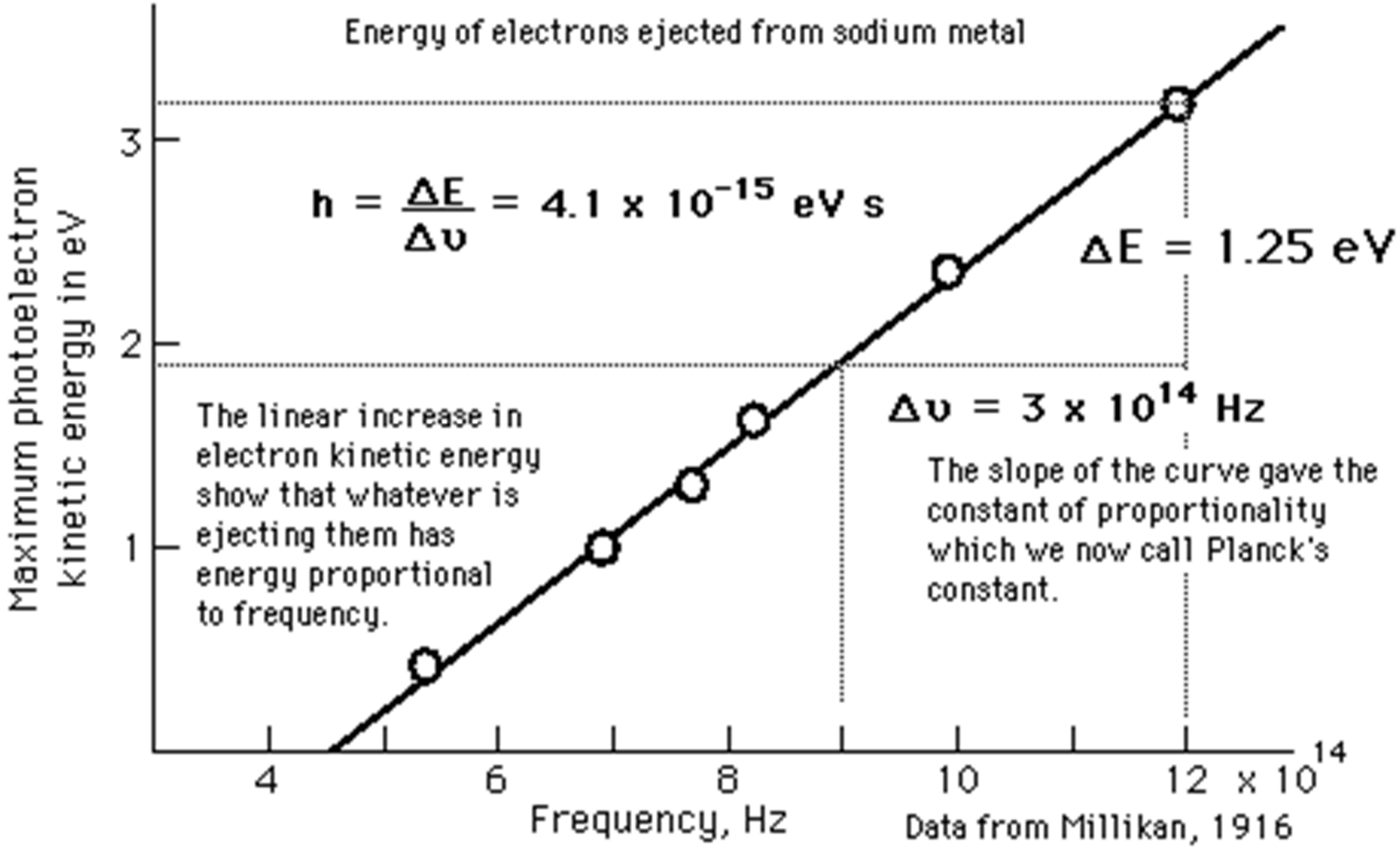


The remarkable aspects of the photoelectric effect when it was first observed were:

1. The electrons were emitted immediately - no time lag!
2. Increasing the intensity of the light increased the number of photoelectrons, but not their maximum kinetic energy!
3. Red light will not cause the ejection of electrons, no matter what the intensity!
4. A weak violet light will eject only a few electrons, but their maximum kinetic energies are greater than those for intense light of longer wavelengths!

A. Einstein : quantification of ligth ennergy (photon) ⇔ $E = nh\nu$, ligth is like a grain (ball) of light ⇔ *corpuscular aspect* !!

The end of the classical mechanics?

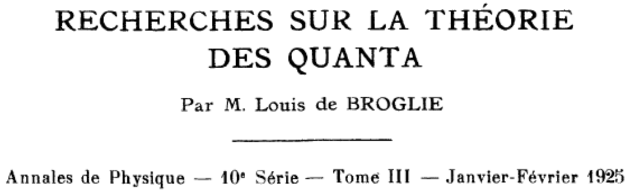


The end of the classical mechanics?

- New experiences / discoveries pose problems of interpretation:
  - Wave – particle duality: particle nature(photoelectric effect) of light is accepted but its wave nature is also accepted (double slit experiences - Young)!
  - The ligth is composed with a quatum, a quantic particle wich can not be described only by the new mechanics: the wave mechanics is born.
  - Dependint of experience, we can use the wave descripton of the light (light propoagation) or particle aspects (light – particle interaction).

The end of the classical mechanics?

- New experiences / discoveries pose problems of interpretation:
  - Louis de Broglie: new concepts of waves of matter. (1924)
  - Hypothesis: wave particle duality is a general propertie of *microscopics objects* and the matter, as light, shows in the same time, wave property and particle property.
  - This hypothesis is confirmed few years later by the diffraction of electrons. (1927).



RECHERCHES SUR LA THÉORIE
DES QUANTA

Par M. Louis de BROGLIE

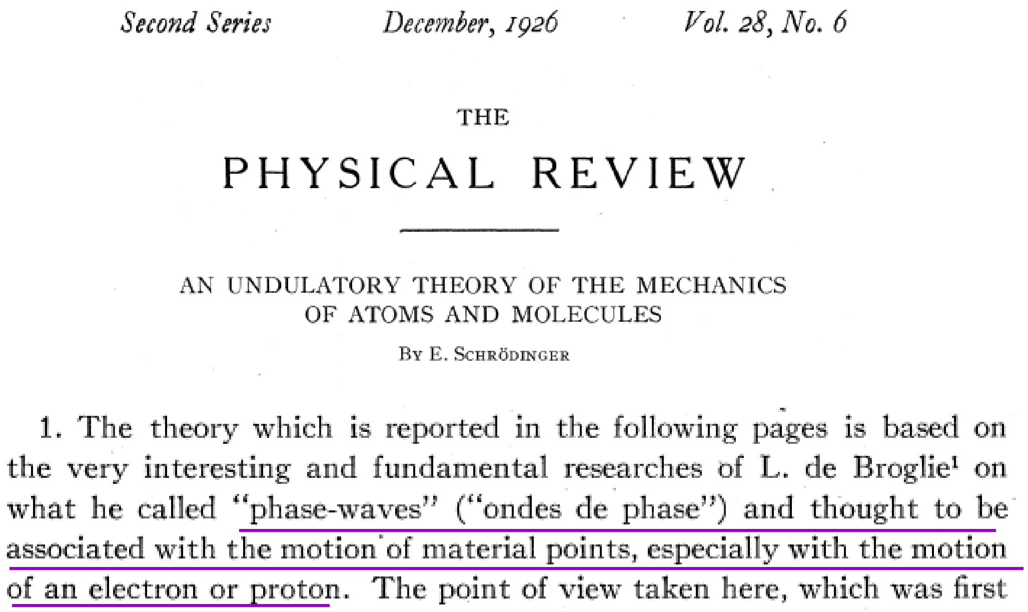
Annales de Physique — 10ᵉ Série — Tome III — Janvier-Février 1925

Waves of matter ⇔ de Broglie wavelength :

$$\boxed{\lambda = \frac{h}{mv} = \frac{h}{p}}$$

Wave mechanics

- *The relation of de Erwin Schrödinger:*



Second Series *December, 1926* *Vol. 28, No. 6*

THE
PHYSICAL REVIEW

AN UNDULATORY THEORY OF THE MECHANICS OF ATOMS AND MOLECULES

BY E. SCHRÖDINGER

1. The theory which is reported in the following pages is based on the very interesting and fundamental researches of L. de Broglie[1] on what he called "phase-waves" ("ondes de phase") and thought to be associated with the motion of material points, especially with the motion of an electron or proton. The point of view taken here, which was first

Wave mechanics

- *the relation of Schrödinger:*

  the motion of a particle is described by a wave function $\Psi(r,t)$ and the norm squared of this function represents the probability of presence or density on a point r. the functions $\Psi(r,t)$ obey to the Schrödinger's relation:

$$-\frac{\hbar^2}{2m}\Delta\Psi(r,t)+V(r,t)\Psi(r,t)=i\hbar\frac{\partial\Psi(r,t)}{\partial t}$$

  - $\Psi(r,t)$ is the wave function (can be a complex quantity)
  - $V(r)$ is the ***potentiel energy*** applied to the particle
  - m is the mass of the particle

- *The relation of Schrödinger:*
  - *Taking into account the quanta notion (Planck) but also the wave-particle duality (de Broglie)*

Wave mechanics

- One particular point for this lecture is concerning steady state (stationary state) where the potential energy V=V(r) applied to the particle is time independent. We have to determine the time-dependent portion and the position-dependent by using the technique of separation of variables. We assume that we can write the wave function:

$$\Psi(r,t)=\varphi(r)\chi(t)$$

  - $\varphi(r)$ is only position dependent
  - $\chi(t)$ is only time dependent

- Susbtituting this form of the solution into Schrödinger's wave equation, we obtain (one dimension approximation):

$$-\frac{\hbar^2}{2m}\frac{1}{\varphi(x)}\frac{\partial^2\varphi(x)}{\partial x^2}+V(x)=i\hbar\frac{1}{\chi(t)}\frac{\partial\chi(t)}{\partial t}$$

Schrödinger equation:

$$-\frac{\hbar^2}{2m}\underbrace{\frac{1}{\varphi(x)}\frac{\partial^2\varphi(x)}{\partial x^2}}_{g(x)}+V(x)=i\hbar\underbrace{\frac{1}{\chi(t)}\frac{\partial\chi(t)}{\partial t}}_{f(t)}$$

- Since the left side is a function of position *x* only and the right side is a function of time *t* only, the only solution is that the both terms are equal to a constant. On the other hand, we see by dimensional analysis of the right side that the constant is an energy:

$$i\hbar\frac{1}{\chi(t)}\frac{\partial\chi(t)}{\partial t}=E \quad\Rightarrow\quad \chi(t)=Ae^{-i\frac{E}{\hbar}t}$$

- Avec *E*, total energy of the particle: $E=\hbar\omega$

Schrödinger equation:

- The time independent part of Schrödinger equation can be writen as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}+V(x)\varphi(x)=E\varphi(x)$$

  - with : $\psi(x,t)=\varphi(x)\exp(\frac{-iE}{\hbar}t)$

- Limits boudaries: $\int_{-\infty}^{+\infty}|\varphi(x)|^2\,dx=1$

  - Continuity of the wave function
  - Continuity of the first derivative

Schrödinger’s equation:

⚠

- At this stage, it is important to distinguish the concept of wave state (plane wave) and combination of wave states (wave packet)

Plane wave/ wave packets

- Plane wave:

$$Ae^{ikx}e^{-i\omega t}$$

- Wave packets:

$$\varphi(x,t) = \int_{k_0-\Delta k/2}^{k_0+\Delta k/2} Ae^{ikx}e^{-i\omega t}\,dk$$

- We will show that only the waves packet can be a good representation of a particle

Plane wave/ wave packets

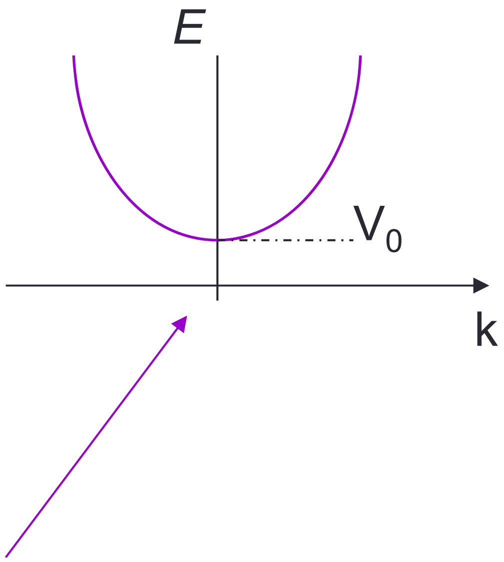
- We suppose a particle are travelling in a constant potential energy $V(x) = V_0$ = cte. It is subjected to a force given by a F = - grad $V_0 = 0$. it means that its motion is uniform and its energy *E is a constant*. We'll now:

  - Find simple solutions of the E.S (plane wave)
  - Verify that these solutions have a physics reality
  - If not, we'll try a linear combination (wave packet) of simple solutions (note that Equation of Schrödinger is a Linear equation with φ)

Plane wave/ wave packets

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}+V_0\varphi(x)=E\varphi(x)$$

$$\frac{\partial^2\varphi(x)}{\partial x^2}+\frac{2m(E-V_0)}{\hbar^2}\varphi(x)=0\ ,\ E-V_0>0$$



One simple solution can be found *φ(x)*: $\varphi(x)=Ae^{ikx}$

with $k=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ or $E=\frac{\hbar^2k^2}{2m}+V_0$

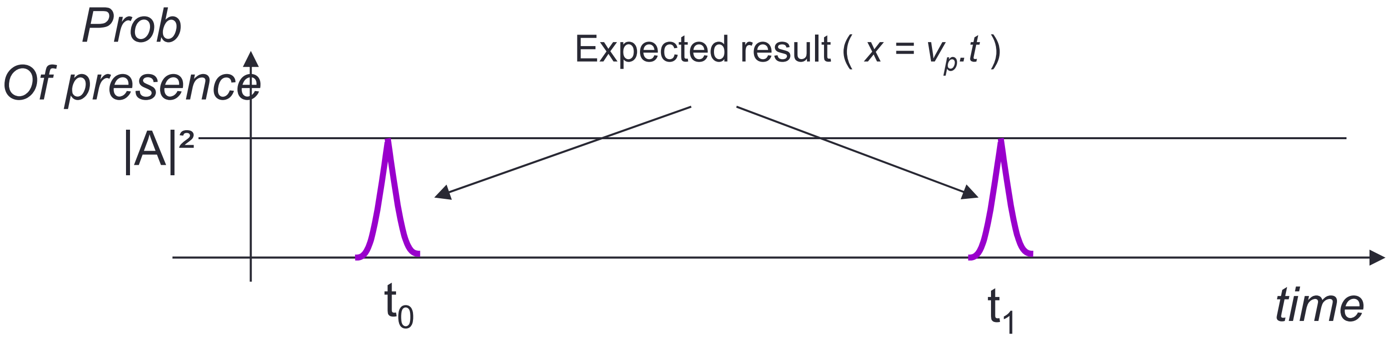
The question is *"Can we represent a particle by this function?".* You only have to *calculate the probability of presence in space (or in 1D)* of this particle to answer this question

Plane wave/ wave packets

- *Plane wave:*

$$\psi(x,t) = Ae^{ikx}e^{-i\omega t}$$

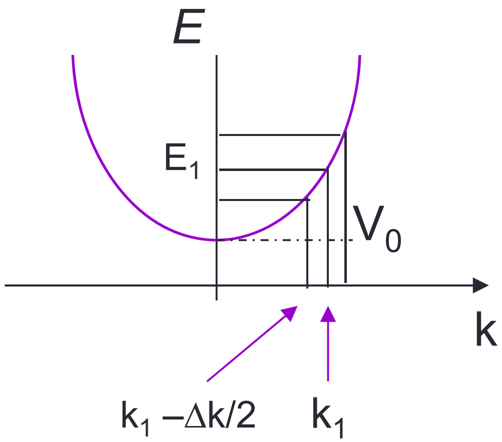
$$\left|\psi(x,t)\right|^2 = \left(\psi(x,t)\psi^*(x,t)\right)^2 = \left|A\right|^2 = cste$$



- *the probability of presence is independent of x and time, which is far from being "reasonable" from a physical point of view*

Plane wave/ wave packets

- So we will try a linear combination of plane waves centered on k_1 ie a wave packet from $k_1 - \Delta k/2$ and $k_1 + \Delta k/2$. The wave function can be written



$$\Psi(x,t) = \int_{k_1-\Delta k/2}^{k_1+\Delta k/2} A e^{ikx} e^{-i\omega t} dk$$

- We suppose A=cste (hyp)
  - at t=0:

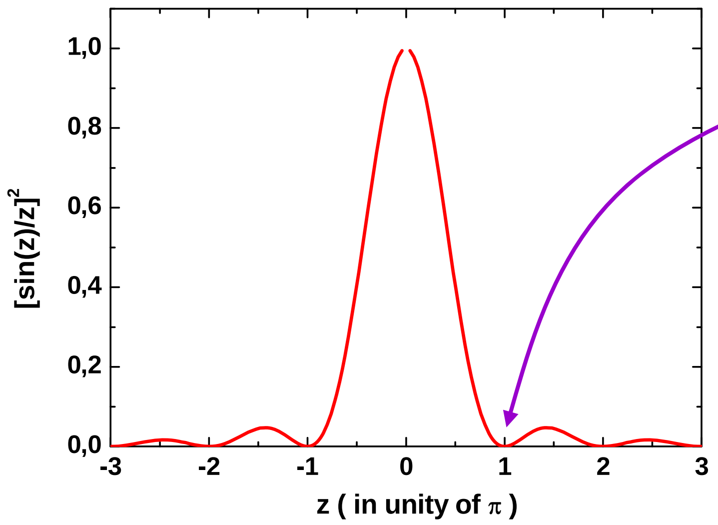
$$\Psi(x,0) = \int_{k_1-\Delta k/2}^{k_1+\Delta k/2} A e^{ik_1x} e^{i(k-k_1)x} dk = A e^{ik_1x} \int_{-\Delta k/2}^{\Delta k/2} e^{i(k-k_1)x} d(k-k_1)$$

$$\Psi(x,0) = A e^{ik_1x} . \frac{1}{ix} \left[e^{i(k-k_1)x} \right]_{-\Delta k/2}^{\Delta k/2} = A e^{ik_1x} \Delta k \frac{\sin(\Delta k x/2)}{\frac{\Delta k}{2} x}$$

Plane wave/ wave packets

- We calculate again the probability of presence at x:

$$\left|\Psi(x,0)\right|^2 = A^2 \Delta k^2 \frac{\sin^2 z}{z^2} \quad \text{avec}\ z = \frac{\Delta k \times x}{2}$$



$$x_1 = \pm \frac{2\pi}{\Delta k} \Rightarrow \Delta x = 2x_1 \approx \frac{4\pi}{\Delta k}$$

$$\Leftrightarrow \Delta x \times \Delta k \approx 4\pi$$

By improving the law of amplitude (instead of A=cte) , one would get the Heisenberg's equation:

$$\boxed{\Delta x \times \Delta k \approx 2\pi}$$

Plane wave/ wave packets

- At t=t$_1$:

$$\Psi(x,t_1)=\int_{k_1-\Delta k/2}^{k_1+\Delta k/2} Ae^{-i\omega_k t_1}e^{ikx}dk = Ae^{ik_1x}e^{-i\omega_1 t_1}\int_{-\Delta k/2}^{\Delta k/2} e^{i(k-k_1)x}e^{i(\omega_k-\omega_1)t_1}d(k-k_1)$$

$$Taylor\ series:\ \omega_k=\omega_1+\left(\frac{d\omega_k}{dk}\right)_{k_1}(k-k_1)+\ldots$$

$$\Psi(x,t_1)=Ae^{ik_1x}e^{-i\omega_1 t_1}\int_{-\Delta k/2}^{\Delta k/2} e^{i(k-k_1)x}e^{i(k-k_1)\left(\frac{d\omega_k}{dk}\right)_{k_1}t_1}d(k-k_1)$$

$$\text{we take}\quad x'=x-\left(\frac{d\omega_k}{dk}\right)_{k_1}t_1 \Rightarrow \Psi(x,t_1)=Ae^{ik_1x}e^{-i\omega_1 t_1}\int_{-\Delta k/2}^{\Delta k/2} e^{i(k-k_1)x'}d(k-k_1)$$

$$\boxed{\Psi(x,t_1)=Ae^{ik_1x}e^{-i\omega_1 t_1}\times\frac{e^{\frac{\Delta k}{2}x'}-e^{-\frac{\Delta k}{2}x'}}{ix'}=B\Delta k\frac{\sin\frac{\Delta k}{2}x'}{\frac{\Delta k}{2}x'}\ \text{avec}\ \frac{\Delta k}{2}x'=\frac{\Delta k}{2}x-\frac{\Delta\omega}{2}t_1}$$

Plane wave/ wave packets

- we get the same result when t = 0 but for x’ = 0, ie

$$x = \left(\frac{d\omega}{dk}\right)_{k_1} t_1$$

The velocity of the particle = v_g = group velocity which is calculated at the center of the wave packet:

$$v_g = \left(\frac{d\omega}{dk}\right)_{k_1}$$

Phase velocity/ group velocity

- In the case of a plane wave, the velocity is the propagation velocity of planes in phase or phase velocity :

$$v_\varphi = \frac{\omega}{k} \quad \left(k = \frac{2\pi}{\lambda} = \frac{2\pi}{v_\varphi T} = \frac{\omega}{v_\varphi}\right)$$

$$\text{from de Broglie} \left(p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k\right)$$

$$v_\varphi = \frac{\omega}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p} = \frac{E}{\hbar k} \quad \text{or } E = \frac{\hbar^2 k^2}{2m} + V_0$$

$$\boxed{\Rightarrow v_\varphi = \frac{1}{2}\frac{\hbar k}{m} + \frac{V_0}{\hbar k} = \frac{1}{2}\frac{p}{m} + \frac{V_0}{p}}$$

this term should not exist (!)
V_0=cst ⇔ no action on the motion of the particle; absurd because $v_\varphi = p/m$

- reasoning on the wave packet:

$$E = \frac{\hbar^2 k^2}{2m} + V_0$$

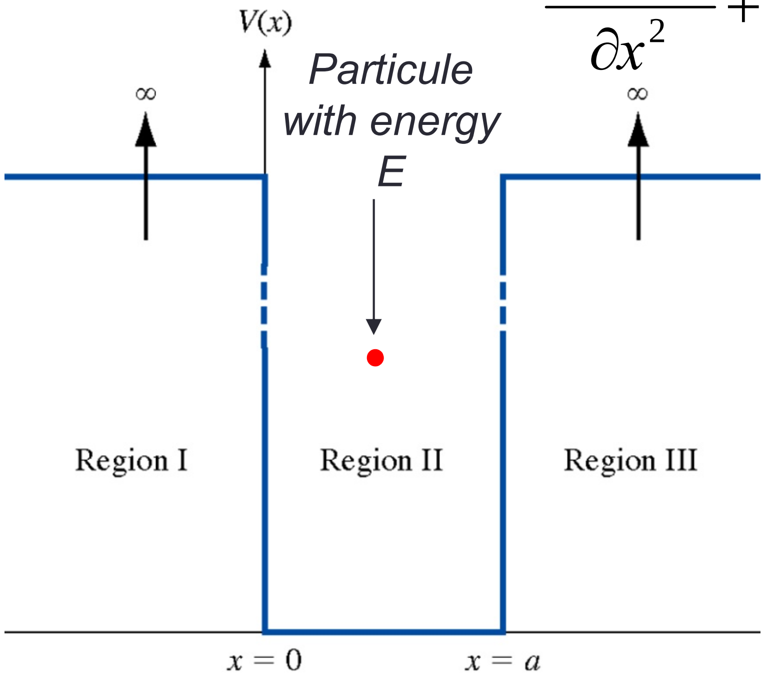
$$\left(\frac{dE}{dk}\right)_{k_1} = \hbar\left(\frac{d\omega}{dk}\right)_{k_1} = \frac{\hbar^2 k_1}{m} \Rightarrow v_g = \frac{p_1}{m}$$

$$\Rightarrow \text{We get } v = \frac{p}{m}$$

Wave Equation: applications of Schrödinger's equation

- *Infinite potential well and width a:*
  - Classical representation of a bound particle.

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\varphi(x) = 0 \quad \text{we set } k = \sqrt{\frac{2mE}{\hbar^2}}$$

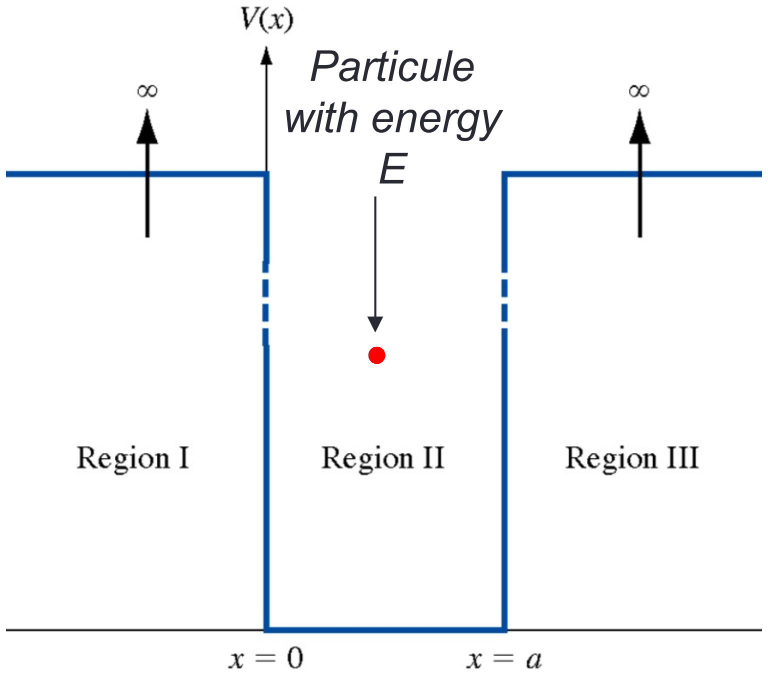


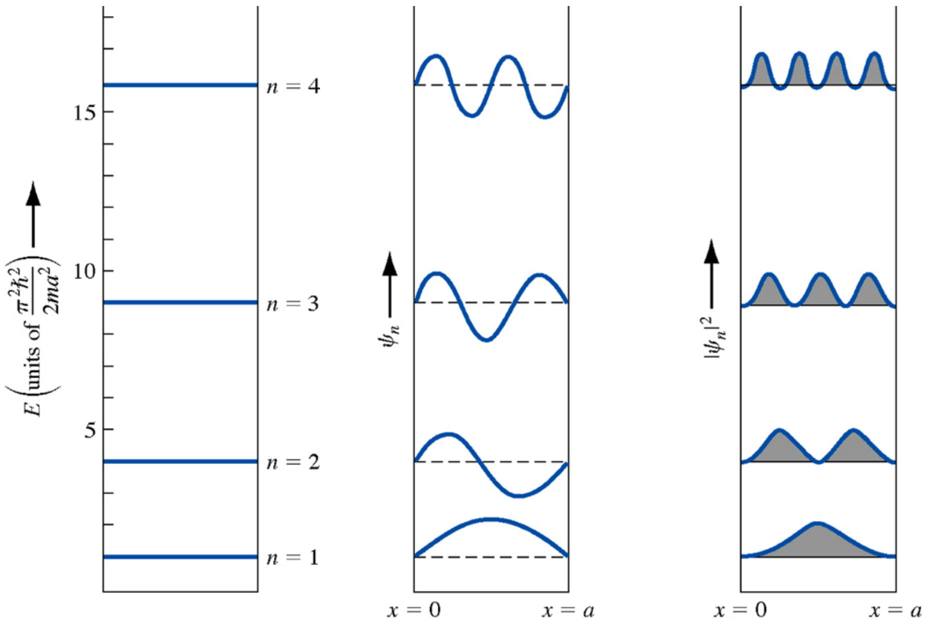
- Region II: $\varphi_{II}(x) = A\cos(kx) + B\sin(kx)$
- Region I et III: $\varphi(x) = 0$
- Continuity at x=0 and x=a
  - A=0
  - $B\sin(ka) = 0 \Leftrightarrow k = n\pi/a$
- probability between 0 and a must be 1:
  - B= $\pm\sqrt{\frac{2}{a}}$ ou $\pm i\sqrt{\frac{2}{a}}$

Wave Equation: applications of Schrödinger's equation

- *Infinite potential well and width a:*

$$\varphi(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad \text{with } n=1,2,3,\ldots \qquad E=E_n=\frac{\hbar^2 n^2 \pi^2}{2ma^2} \quad \text{with } n=1,2,3,\ldots$$


Particule with energy E



(a) (b) (c)

Wave Equation: applications of Schrödinger’s equation

- *The step potential function:*
    - *Region I:*

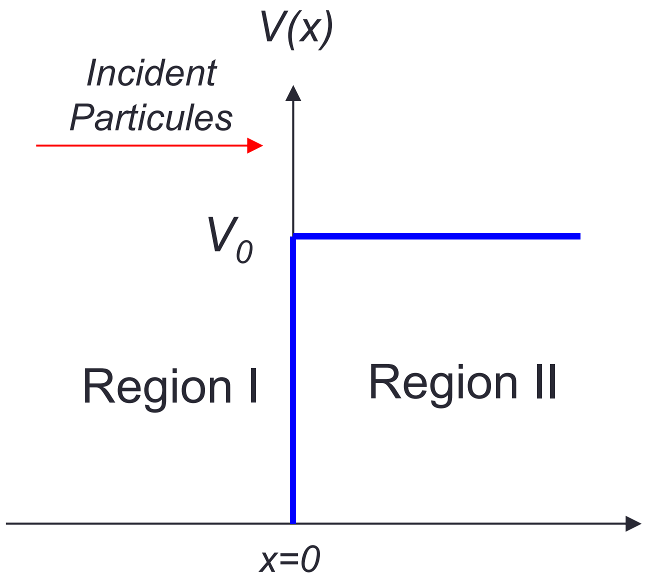
$$\frac{\partial^2 \varphi_1(x)}{\partial x^2} + \frac{2m}{\hbar^2} E\varphi_1(x) = 0$$

- *Region II ($0<E<V_0$)*

$$\Rightarrow \varphi_1(x) = A_1 e^{ikx} + \underline{B_1 e^{-ikx}} \quad \text{avec}\; k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{\partial^2 \varphi_2(x)}{\partial x^2} - \frac{2m}{\hbar^2} (V_0 - E)\varphi_2(x) = 0$$

$$\Rightarrow \varphi_2(x) = A_2 e^{\rho x} + B_2 e^{-\rho x} \quad \text{avec}\; \rho = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$



Wave Equation: applications of Schrödinger's equation

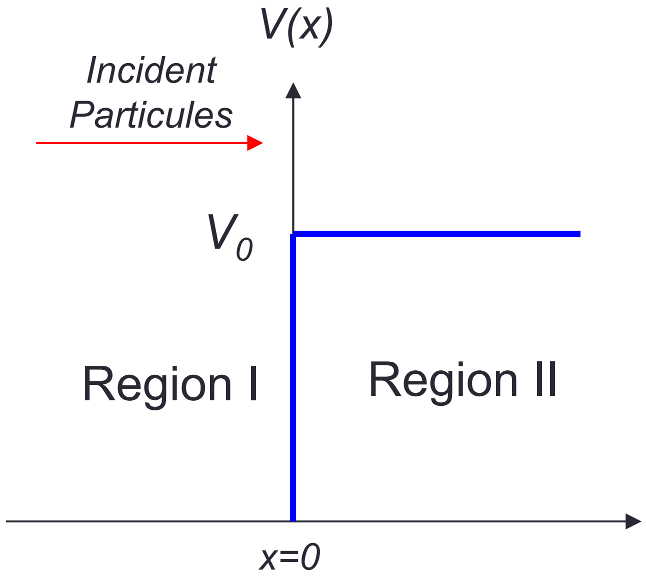
- *The step potential function*
  - $A_2 = 0$ (divergence)
  - *Reflexion coefficient:*

Flux of reflected particles ($cm^{-2}\ s^{-1}$)

$$R = \frac{v_r}{v_i}\frac{B_1 B_1^*}{A_1 A_1^*} = \frac{v_r}{v_i}\left|\frac{B_1}{A_1}\right|^2$$

- *In region I, V=0 ⇔ energy is only cinetic energy*

$$k = \sqrt{\frac{2m}{\hbar^2}\left(\frac{1}{2}mv^2\right)} = \frac{mv}{\hbar} \Rightarrow v_i = v_r = \frac{\hbar}{m}k$$



$$R = 1$$

$\varphi_2(x) \neq 0$ ⇔ particle(in contradiction with classical mechanics) can be present

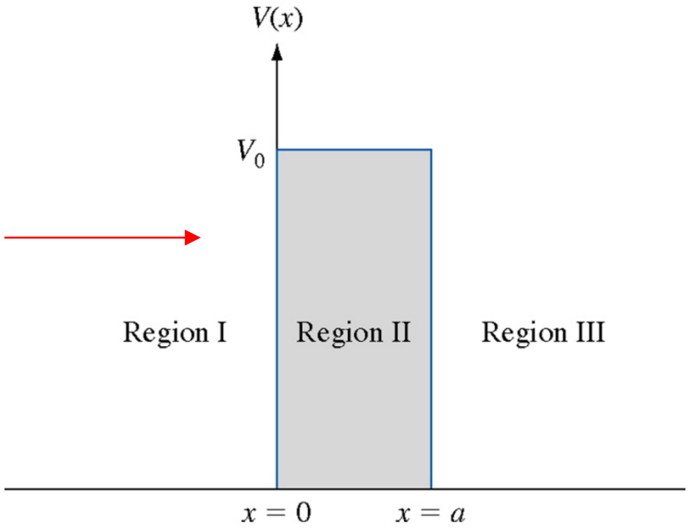
Wave Equation: applications of Schrödinger's equation

- *The Potential barrier ($E<V_0$):*

$$\varphi_1(x) = A_1e^{ikx} + B_1e^{-ikx} \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\varphi_2(x) = A_2e^{\rho x} + B_2e^{-\rho x} \text{ with } \rho = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\varphi_3(x) = A_3e^{ikx} + \cancel{B_3}e^{-ikx}$$



- *Transmission coefficient :*

$$T = \frac{v_t}{v_i}\frac{A_3A_3^*}{A_1A_1^*} = \frac{A_3A_3^*}{A_1A_1^*} = \frac{4E(V_0-E)}{4E(V_0-E)+V_0^2 sh^2\left[\sqrt{2m(V_0-E)}a/\hbar\right]} \neq 0$$

It's tunneling or tunnel effect (T~78% with 1 alectron, $E=V_0/2=1$ev and $a=1$Å)

CHAPTER 4

Free electrons:

model of *Sommerfeld*

Free electron

- Free electron⇔ energy potential is zero everywhere⇔ *V(x)=0:*

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + \frac{2m}{\hbar^2} E\varphi(x) = 0$$

- Solution of this differential equation is given by:

$$\varphi(x) = A\exp\left[\frac{i\sqrt{2mE}}{\hbar}x\right] + B\exp\left[-\frac{i\sqrt{2mE}}{\hbar}x\right]$$

- And :

$$\boxed{\psi(x,t) = \varphi(x)\exp(-i\frac{E}{\hbar}t) = A\exp\left[\frac{i}{\hbar}(x\sqrt{2mE} - Et)\right] + B\exp\left[-\frac{i}{\hbar}(x\sqrt{2mE} + Et)\right]}$$

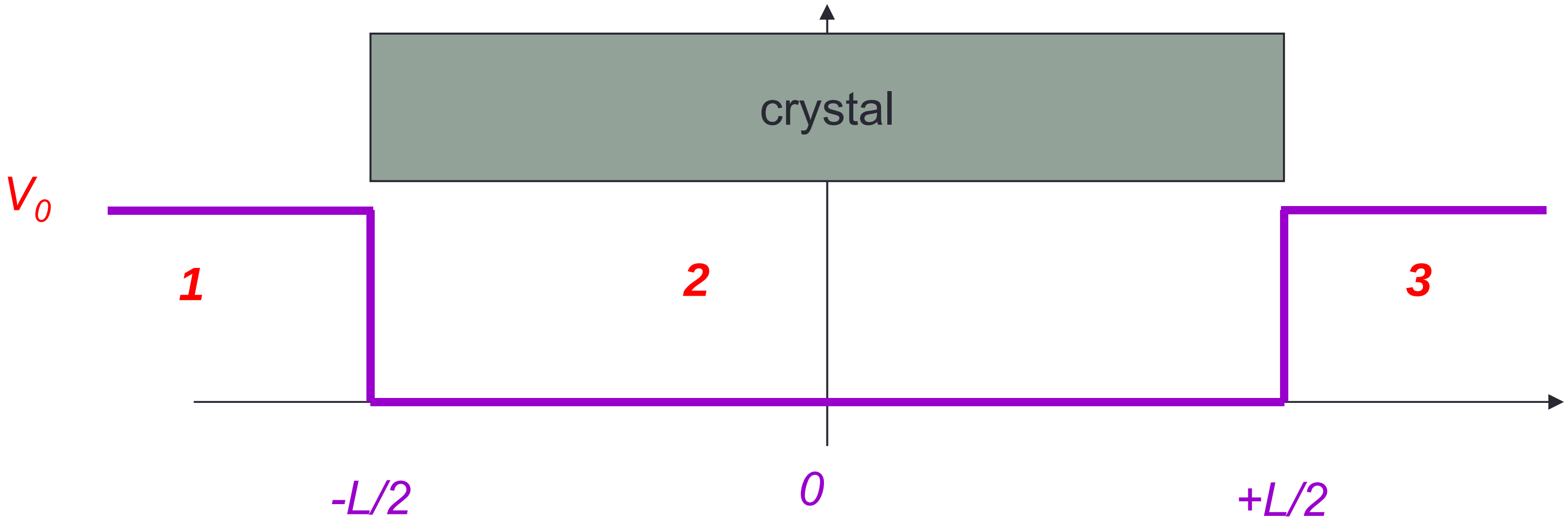
Free electron

$$\psi(x,t)=\varphi(x)\exp(-i\frac{E}{\hbar}t)=A\exp\left[\underbrace{\frac{i}{\hbar}(x\sqrt{2mE}-Et)}_{+\,x}\right]+B\exp\left[\underbrace{-\frac{i}{\hbar}(x\sqrt{2mE}+Et)}_{-\,x}\right]$$

- wave propagation ⇔ a particle in the vacuum can be represented by a wave: this is normal, we started with Schrödinger's equation!
- We suppose for simplicity taht *B=0* ⇔ incident wave only in the positive x
  - *Wave vector*: $k=2\pi/\lambda$
  - *wavelength:* $\lambda=h/\sqrt{2mE}$
  - *Energy:* $E=\hbar^2k^2/2m$ *E(k) represents a parabole*
  - *Probability density*: cste =AA^* ⇔ in accordance with Heisenberg (k known => x unknown) ⇔ physics reality wuth wave packets

Sommerfeld Model

- A. Sommerfeld considers one unidirectional crystal (1D) with length L
- The electrons are bound to the crystal by the Coulomb attraction forces.
- The electrons are trapped ⇔ they can not get out



Sommerfeld potential

- *Simplification*: we get closer to reality by considering that the wave function associated with the electron cancels to the limits (± L / 2) ⇔ electrons can not escape from the crystal
- *steps:*
  - Find solutions of Schrodinger’s equation
  - Keep only those that meet/fit conditions of continuity
  - Built a wave packet for a better representation of reality

Sommerfeld potential

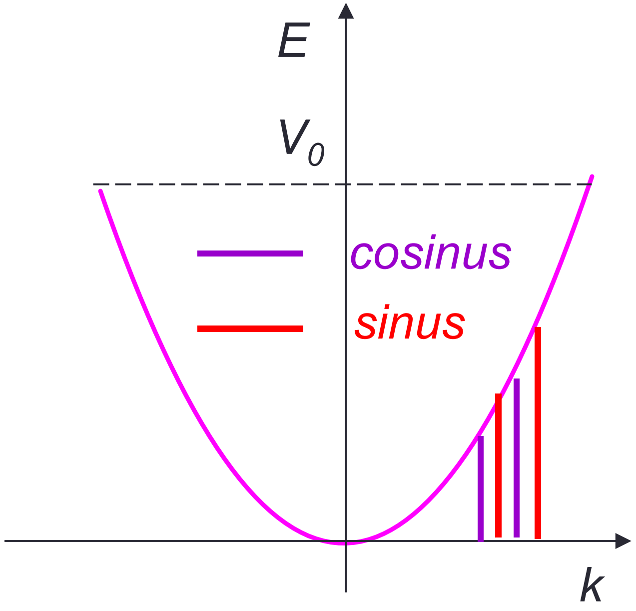
- *Solution for region 2 (idem free electron)*:

$$\frac{\partial^2\varphi(x)}{\partial x^2}+\frac{2m}{\hbar^2}E\varphi(x)=0 \qquad \varphi(x)=Ae^{ikx}$$

$$k=\sqrt{\frac{2mE}{\hbar^2}} \qquad E=\frac{\hbar^2k^2}{2m}$$

- *Continuity conditions:*
  - real: cancel in ± L/2

$$\frac{Ae^{ikx}+cc}{2} \quad \Downarrow \quad A\cos(kx) \qquad\qquad \frac{Ae^{ikx}-cc}{2} \quad \Downarrow \quad A\sin(kx)$$



- Cosinus solutions

$$\cos k\frac{L}{2}=0\Rightarrow k=(2p+1)\frac{\pi}{L}\Rightarrow \Delta k=\frac{2\pi}{L}$$

- Sinus solutions

$$\sin k\frac{L}{2}=0\Rightarrow k=p\frac{2\pi}{L}\Rightarrow \Delta k=\frac{2\pi}{L}$$

Wave vector is quatified
⇔ Energy too !!

Sommerfeld potential

- :*Born–von Karman boundary condition (BVK condition)*
  - The idea is to consider that at the scale of electronic wavelength, the crystal size is infinite ⬄ we assimilates the one-dimensional crystal of length L to a circle of perimeter L: we "forget" the boundary conditions
  - The position at *x* and *x*+*L* is the same:

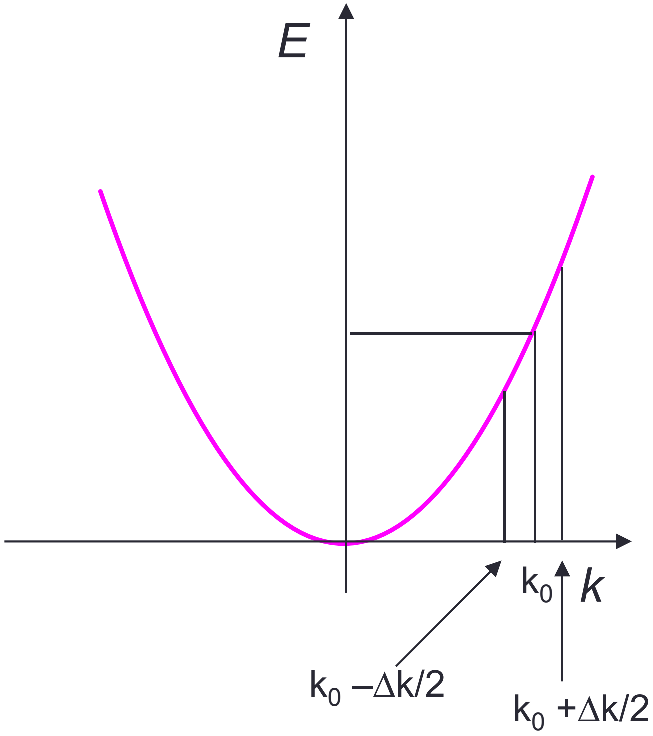
$$\left.\begin{aligned} &e^{ikx} = e^{ik(x+L)} \\ &e^{ikL} = 1 \Rightarrow kL = p \times 2\pi \\ &\Rightarrow k = p\frac{2\pi}{L} \end{aligned}\right\}$$

We get the previous result : k and E are again quantified

Sommerfeld potential

- Sommerfeld Electron:
  - Suppose electron at k_0: the order of L is 10^8Å (1 cm) ⇔ we assume that the wave packet with a width Δk can be considered as a continuum because:

$$\Delta k = \frac{2\pi}{L} = \frac{2\pi}{10^8} \approx 10^{-7} /\overset{\circ}{A}$$



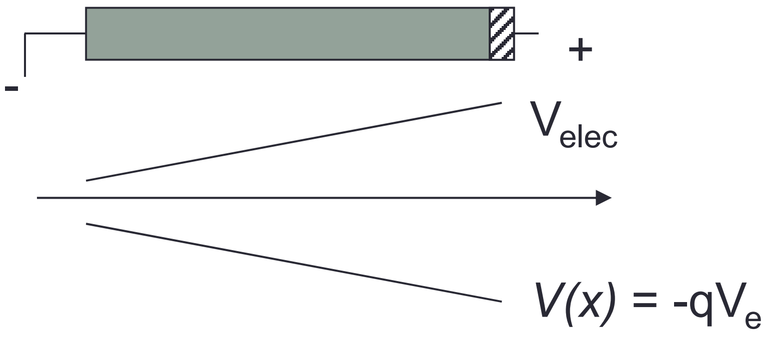
  - *Electron velocity*:

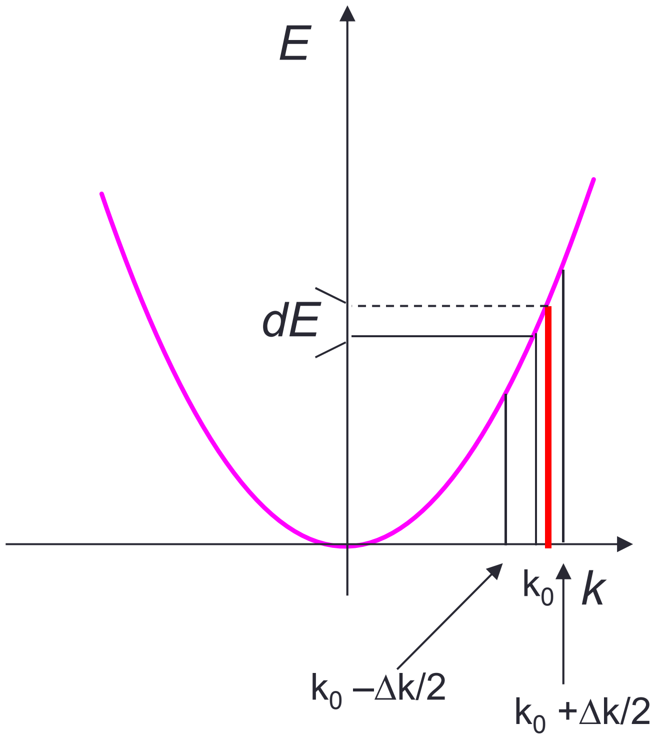
$$v_g = \left(\frac{d\omega}{dk}\right)_{k_0} \quad \text{and } E = \hbar\omega = \frac{\hbar^2 k^2}{2m}$$

$$\Rightarrow v_g = \frac{\hbar k_0}{m} = \frac{p_0}{m}$$

Sommerfeld potential

- Sommerfeld electron:
  - *Electron acceleration:*





The state (electron) gains energy:

⇔ between t and t+dt =>$dE=F.v_g.dt$

⇔ IfiE changes, k must change ⇔ the central value of k_0 is changed (-).

$$dE = F \times v_g \times dt = \left(\frac{dE}{dk}\right)_{k_0} dk = F\frac{1}{\hbar}\left(\frac{dE}{dk}\right)_{k_0} dt = dE$$

$$\Rightarrow F \boxed{= \hbar\frac{dk_0}{dt} = \frac{dp_0}{dt}}$$

Sommerfeld potential

- Sommerfeld electron:
  - *Electron Accélération :*

$$\frac{F}{m} = \frac{dv_g}{dt} = \gamma \quad \text{and} \quad \vec{F} = -\underbrace{\overrightarrow{gradV_0}}_{(=0,\ V_0=\text{cste})} + \underbrace{F_{ext}}_{-qE_{elec}}$$

$$\frac{dv_g}{dt} = -qE_{elec} \quad \text{and} \quad v_g = \left(\frac{d\omega}{dk}\right)_{k_0} = \frac{1}{\hbar}\left(\frac{dE}{dk}\right)_{k_0}$$

$$\frac{dv_g}{dt} = \frac{dv_g}{dk}\frac{dk}{dt} = \gamma$$

$$\gamma = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)_{k_0}\frac{dk}{dt} = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)_{k_0} F = \frac{F}{m}$$

$$\Uparrow$$

$$F = \hbar\frac{dk_0}{dt}$$

If we define:

$$\frac{1}{m} = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)_{k_0} \quad \text{because} \quad E = \frac{\hbar^2k^2}{2m} + V_0$$

$$\Downarrow$$

$$\boxed{\frac{dv_g}{dt} = \gamma = \frac{F}{m} \quad \text{avec} \quad \frac{1}{m} = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)_{k_0}}$$

Sommerfeld potential

$$\frac{dv_g}{dt} = \gamma = \frac{F}{m} \quad \text{avec} \quad \frac{1}{m} = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)_{k_0}$$

- Nota: the relationship F = mg is always true. The calculated mass is the mass of the particle only if that V = V0 = constant, ie that the resultant forces are equal to the external forces. For a potential V (x) which is not constant, the relationship is the same if we replace the mass by an effective mass (m*) that will reflect a response different (inertia different due to potentiel energy) compare to a free particle (see below!)

Wave theory applied to atoms: the Bohr – Sommerfeld atom

- Atom with one eletron (Hydrogen):
  - nucleus « heavy », positively charged (proton)
    - It is immobile
  - Electron is « ligth », negatively charged
  - Coulomb attraction between electron and proton is given by:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

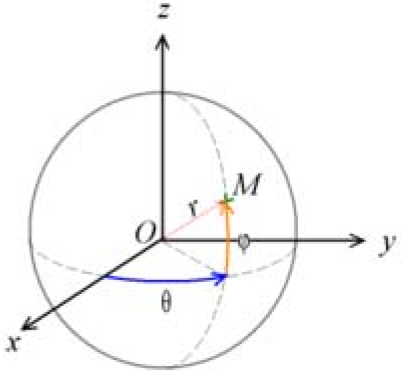
- *e* : electronic charge
- ε_0 : permitivity of free space

→ *Leads to a 3D problem of Schrödinger equation*

Bohr – Sommerfeld atom

- *3D Schrödinger equation (sperical coordinates)*

$$\nabla^2\varphi(r,\theta,\phi)+\frac{2m_0}{\hbar^2}(E-V(r))\varphi(r,\theta,\phi)=0$$



- *and:*

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\varphi}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\varphi}{\partial r^2}+$$

$$\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\varphi}{\partial\theta}\right)+\frac{2m_0}{\hbar^2}(E-V(r))\varphi=0$$

Bohr – Sommerfeld atom

- We apply the separation of variables technique:

$$\varphi(r,\theta,\phi) = R(r).\Theta(\theta).\Phi(\phi)$$

- We get:

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} + \frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)$$
$$+\, r^2\sin^2\theta\,\frac{2m_0}{\hbar^2}(E-V)=0$$

Function of ϕ only

- We may writte

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = -m^2 \quad \Longrightarrow \quad \Phi = \frac{1}{\sqrt{2\pi}}e^{im\phi} \quad \text{avec} \;\; m = 0,\pm1,\pm2,\ldots$$

Be careful : m is not the mass, is a constant obtained via separation of variables technique

Bohr – Sommerfeld atom

- If we proceed the solving (*irrelevant for this course*) for the two other function, we have to introduce two additional constants *l* and *n. m, l* and *n* are known as quantum number:
  - *n= 1, 2, 3,…* ⇔ *principal quantum number*
  - *l= n-1, n-2,…, 0* ⇔ *azimuthal quantum number*
  - *|m|=l, l-1, …, 0* ⇔ *magnetic quantum number*
- *Main result:*
  - Each set of quantum number corresponds to a quantum state which electron can occupy. We get the well known quantified energy of hydrogen

$$\boxed{E_n = -\frac{m_0 e^4}{(4\pi\varepsilon_0\hbar^2)^2 2n^2} = -\frac{R_y}{n^2} = -\frac{13,6}{n^2}eV}$$

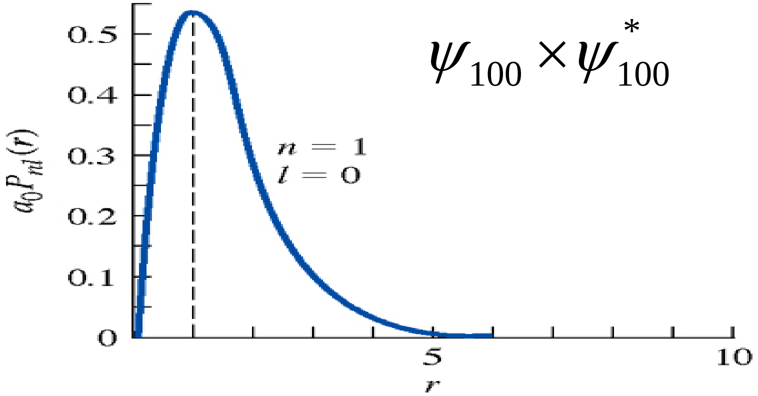
http://scienceworld.wolfram.com/physics/HydrogenAtom.html

Bohr – Sommerfeld atom

- We can show that for the lowest energy state (n=1, l=0 m=0), the wave function is given:

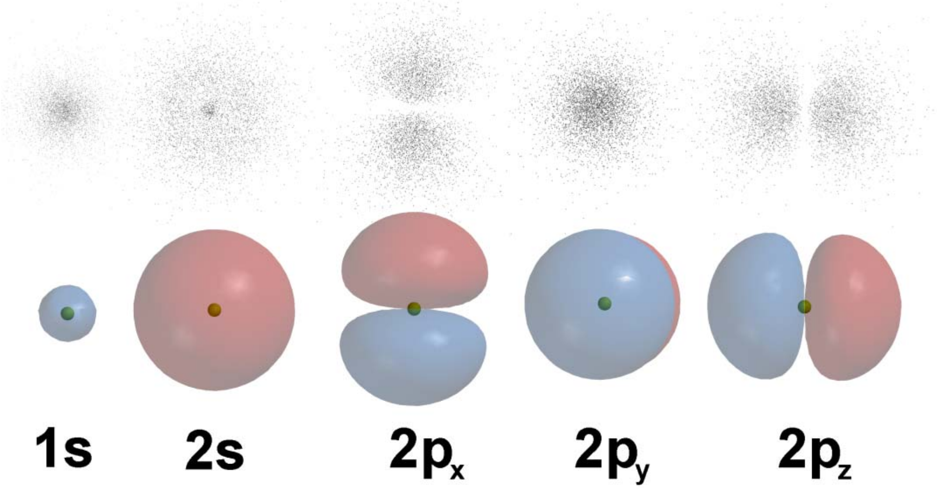
$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_0 e^2} = 0{,}529\ \mathring{A} \quad \text{Bohr radius}$$



$$\psi_{100} \times \psi^*_{100}$$

- *Common writing*:
  - s state l=0
  - p state l=1
  - d state l=2



- *Electronic states*:
  - 1s 2s 2p 3s 3p 3d …

Sommerfeld model

- conclusion:
  - Specific heat explained
  - Ohm’s law explained (see futher)
  - …
  - We can’t explain the difference between the conductivity of an insulator and a metal

$$\frac{\sigma_{metal}}{\sigma_{insulator}} \approx 10^{32} \quad !!!$$

There must be "somewhere" in the model a rough approximation!

CHAPTER 6

Electrons in periodical structure :
Bloch – Brillouin model

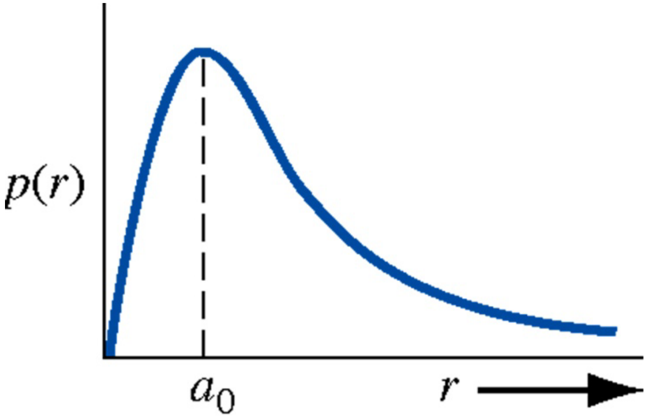
plan

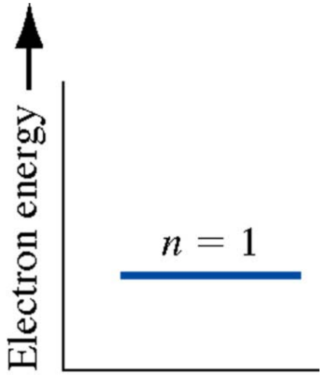
- Formation of energy bands
- Periodicity of the crystal
- Pseudo wave vector or crystal wave vector k
- Bloch waves
- Kronig-Penney model
- Energy band diagram in k space

Formation of energy bands

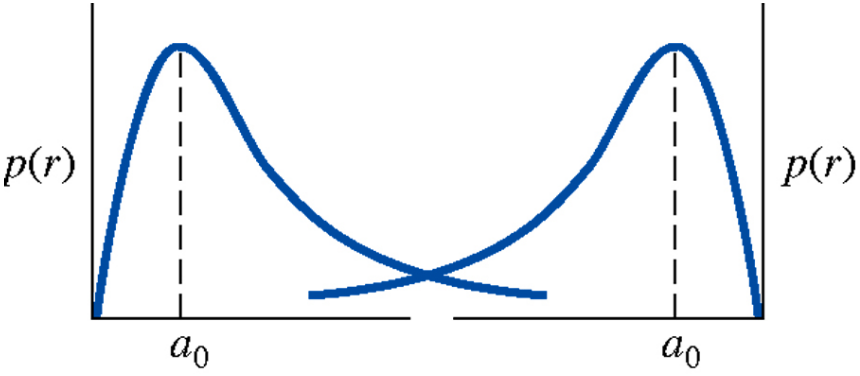
- Qualitative model:

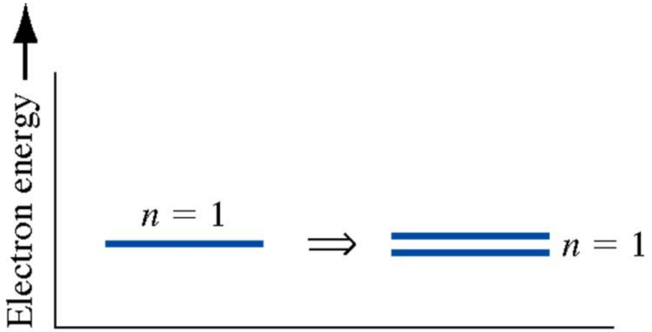
1 isolated hydrogen atom





2 adjacent hydrogen atom



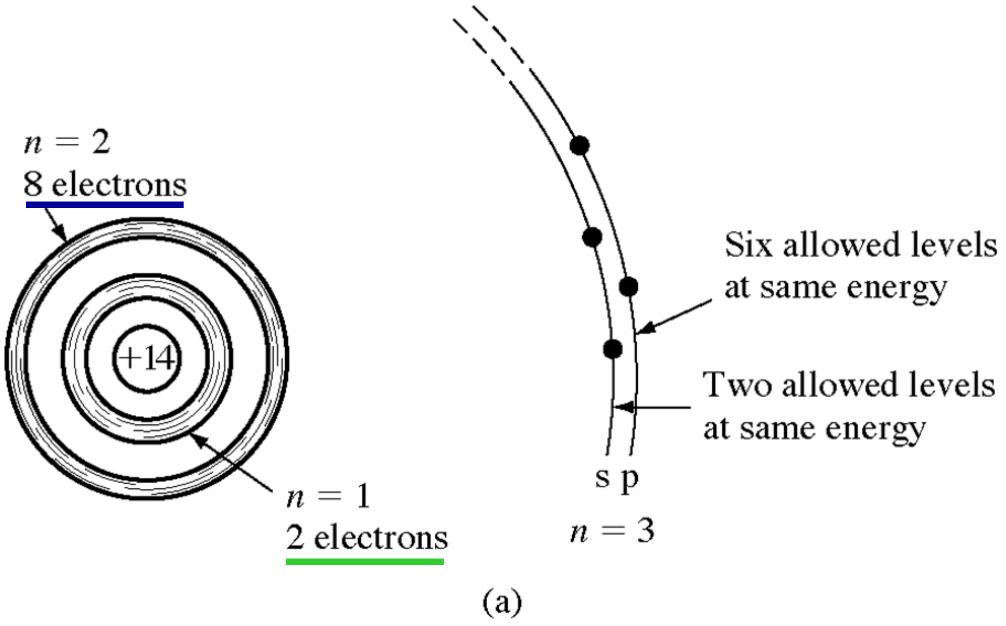


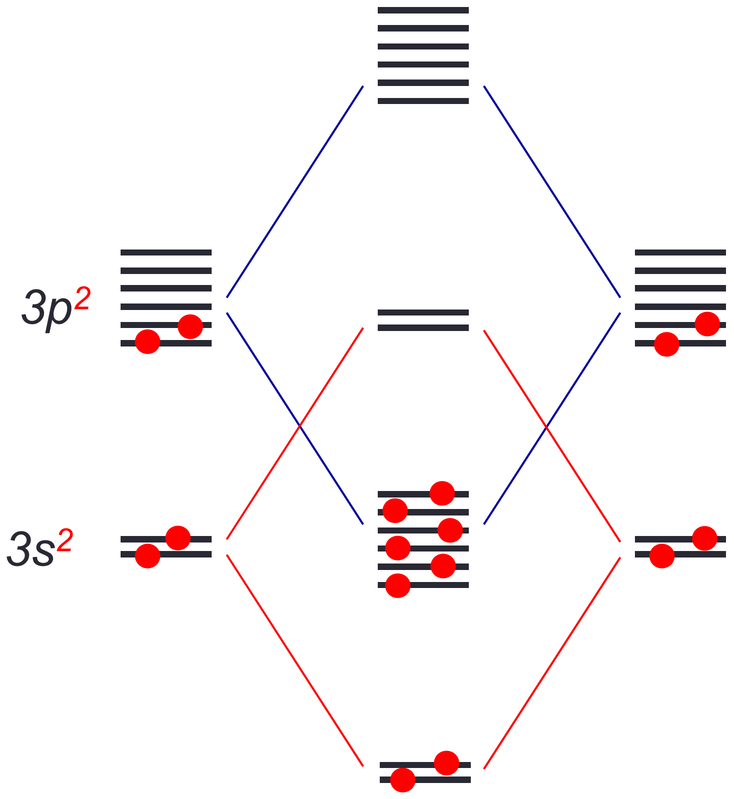
Formation of energy bands

- :Qualitative model for a *Silicon crystal*
  - Electronic structure (14 electrons)
    - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

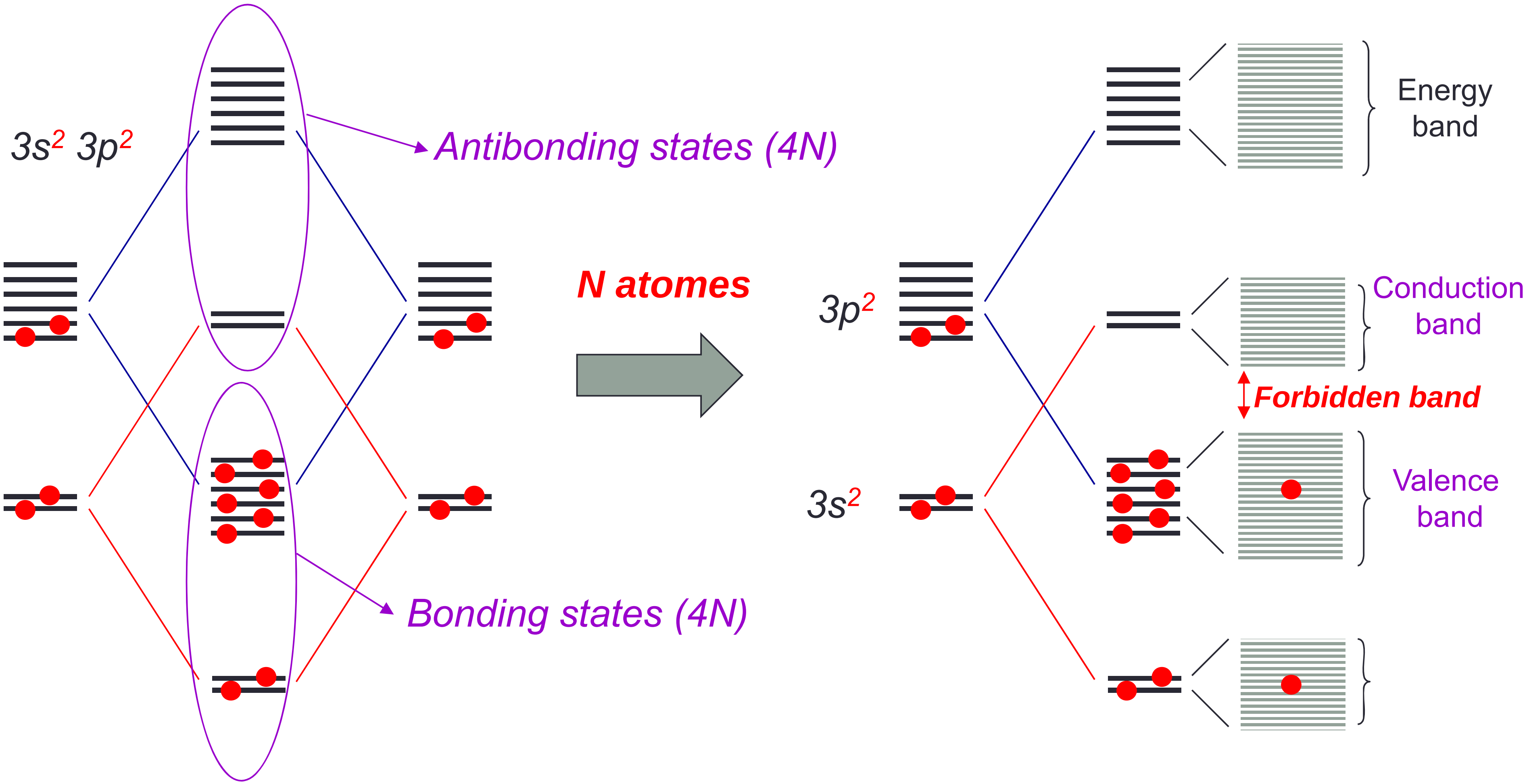
Overlapping

Splitting of energy levels



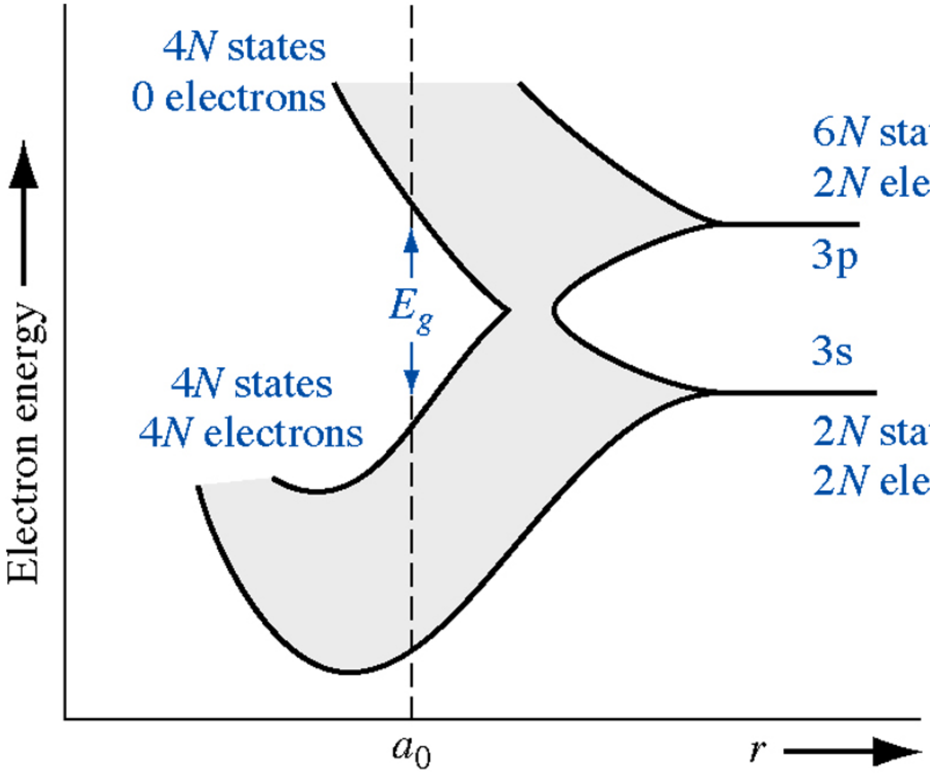


Formation of energy bands



Formation of energy bands

- The value of the forbidden band depends of the equilibrium distance between atoms: a_0

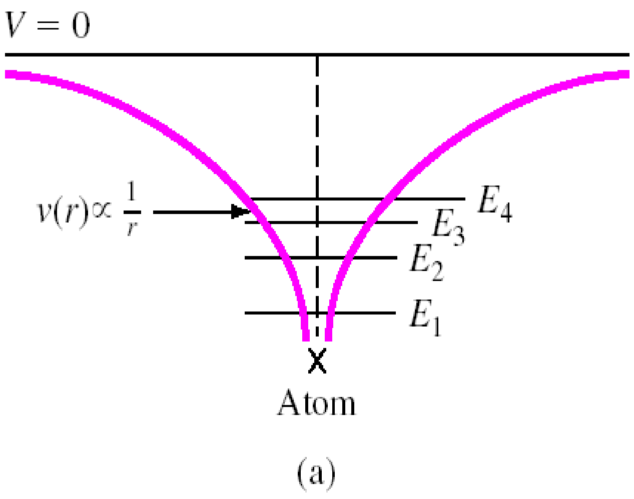


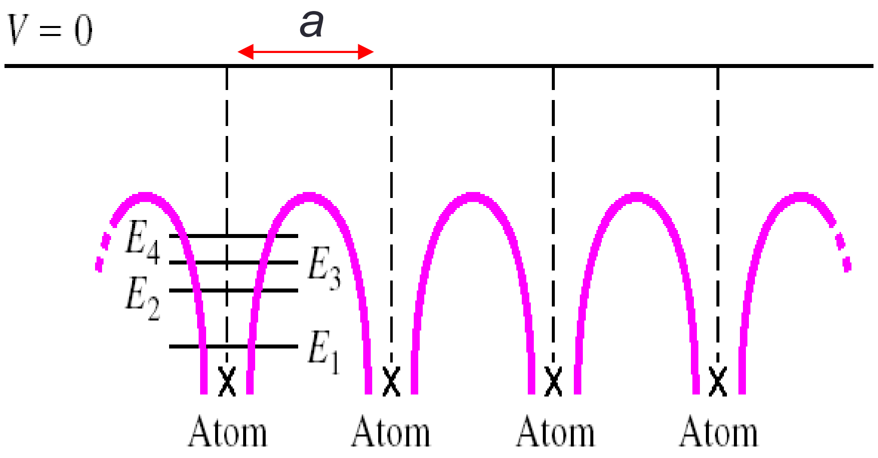
Formation of energy bands

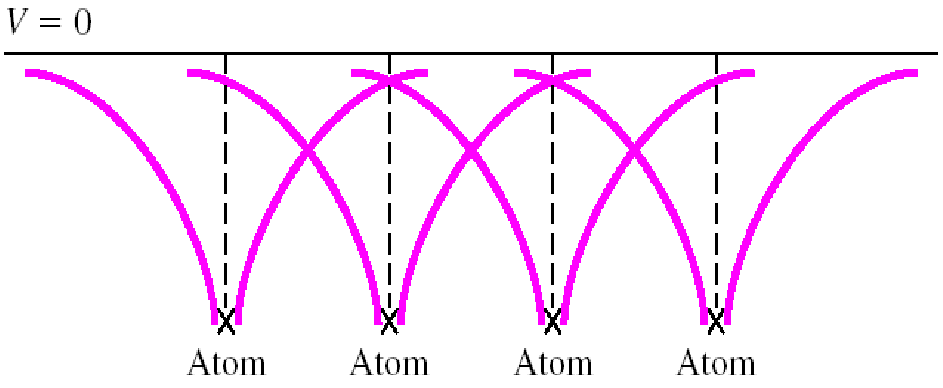
- *Theoritical model using quantum mechanics and Schrödinger eqaution.*
  - *What we have to add /modify to be able to explain/understand the notion of allowed and forbiden energy bands?*

In fact, the crystaline potential where electron is moving is not a constant but it's a periodic function !

Formation of energy bands







(from Neaman)

The crystaline potential (energy) is periodic, with a periode « a

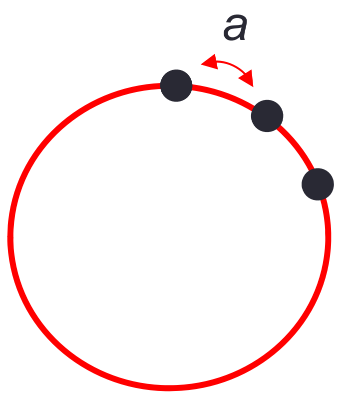
$$V(x) = V(x + a)$$

Bloch Brillouin model

- *BVK condition*: (allows you to ignore what happens at the end of the sample with a length L)
  - Number of Atoms?
    - 1D:
    - 3 D:

$$N = \frac{1}{a} \approx 10^{7}\, cm^{-1}$$

$$N = \frac{1^{3}}{a^{3}} \approx 10^{21}\, cm^{-23}$$



$$\Rightarrow \boxed{\begin{array}{l} V(x+L) = V(x) \\ \psi(x+L) \equiv \psi(x) \end{array}}$$

The crystal being periodic with a period *a*, the crystal properties are the same at x and at x + *a*. It is the same for the wave function, and also for the density probability for the electron.

Bloch Brillouin model

$$dP(x) = \left|\psi(x)\right|^2 \qquad (1)$$

$$dP(x+a) = \left|\psi(x+a)\right|^2 \qquad (2)$$

$$(1) \equiv (2) \qquad \Rightarrow \psi(x)\psi^*(x) = \psi(x+a)\psi^*(x+a)$$

- The two wave functions can be separated by a phase factor:

$$\psi(x+a) = e^{i\theta}\psi(x)\ ,\ \psi(x+2a) = e^{i2\theta}\psi(x), \ldots$$

$$\Rightarrow \psi(x+Na) = e^{iN\theta}\psi(x) = \psi(x)$$

$$\Rightarrow e^{iN\theta} = 1 \quad \Leftrightarrow \quad \boxed{\theta = p\frac{2\pi}{N} = p\frac{2\pi a}{Na} = p\frac{2\pi}{L}a}$$

Bloch Brillouin model

- modification of writing : introduction of *pseudo wave vector or crystal vector K.*
  - We introduce $K = p\dfrac{2\pi}{L}$, so we get:

$$\psi(x+a) = e^{iKa}\psi(x)$$

  - *K* is not a real wave vector, it only represents a phase shift between two waves
  - K is quantified. It takes N values separated by $\dfrac{2\pi}{L}$ and has the same values each $\dfrac{2\pi}{a}$

Bloch Brillouin model

- *Bloch waves:*

$$\psi(x+a)=e^{iKa}\psi(x)=e^{iK(a+x)}e^{-iKx}\psi(x)$$

$$\text{set }\ u(x)=e^{-iKx}\psi(x)\Leftrightarrow\psi(x)=u(x)e^{iKx}$$

and

$$u(x)=e^{-iKx}\psi(x)=e^{-iK(x+a)}e^{iKa}\psi(x)=e^{-iK(x+a)}\psi(x+a)$$

$$\Rightarrow u(x)=u(x+a)$$

- *Stationnary wave functions for an electron in 1D periodic potential must be of the form:*

$$\boxed{\psi(x)=u(x)e^{iKx}\quad\forall x\ \text{ with }\ u(x)=u(x+a)}$$

Bloch Brillouin model

- *Difference plane wave/ Bloch's wave:*
  - Plane wave:

$$\phi(x) = Ae^{ikx} \qquad k = \frac{2\pi}{\lambda} \quad \text{and } \varphi = \frac{2\pi}{\lambda}x$$

  - Bloch's wave:

$$\phi(x) = u(x)e^{iKx} \qquad K = p\frac{2\pi}{L} \quad \text{and } \varphi = Kx + \underbrace{\arg(u(x))}_{\text{unknown}}$$

Bloch Brillouin model

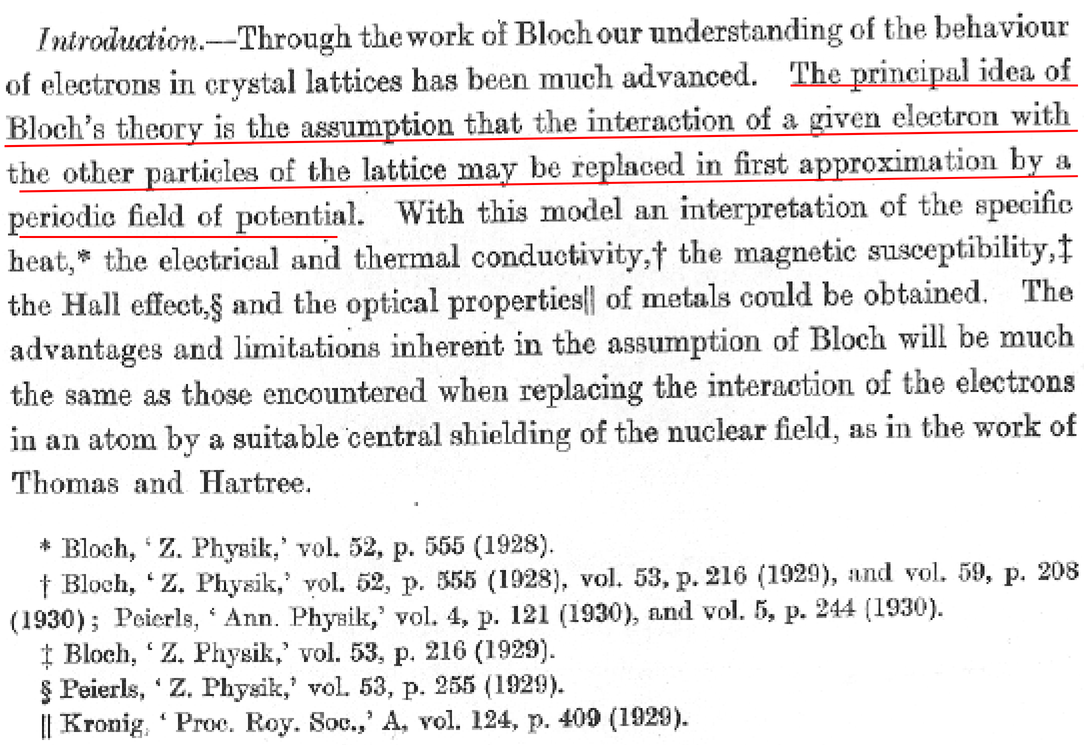
- The Bloch's function has to be injected into the Schrödinger's equation.
  ⇔ for Solving this equation we need to determine *u(x)* !

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(u(x)e^{ikx}\right)+V_0\times u(x)e^{ikx}=E\times u(x)e^{ikx}}$$

- To solve the problem we have to know perfectly the form of the potential energy (not trivial !). A simplified model could give us an idea concerning energy band structure.

Kronig – Penney model

R.D. Kronig and W.G. Penney, "Quantum Mechanics of Electrons in Crystal Lattices",
Proceedings of the Royal Society London **130**, 499 (1931)



Introduction.—Through the work of Bloch our understanding of the behaviour of electrons in crystal lattices has been much advanced. The principal idea of Bloch's theory is the assumption that the interaction of a given electron with the other particles of the lattice may be replaced in first approximation by a periodic field of potential. With this model an interpretation of the specific heat,* the electrical and thermal conductivity,† the magnetic susceptibility,‡ the Hall effect,§ and the optical properties‖ of metals could be obtained. The advantages and limitations inherent in the assumption of Bloch will be much the same as those encountered when replacing the interaction of the electrons in an atom by a suitable central shielding of the nuclear field, as in the work of Thomas and Hartree.

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* Bloch, ' Z. Physik,' vol. 52, p. 555 (1928).

† Bloch, ' Z. Physik,' vol. 52, p. 555 (1928), vol. 53, p. 216 (1929), and vol. 59, p. 208 (1930); Peierls, ' Ann. Physik,' vol. 4, p. 121 (1930), and vol. 5, p. 244 (1930).

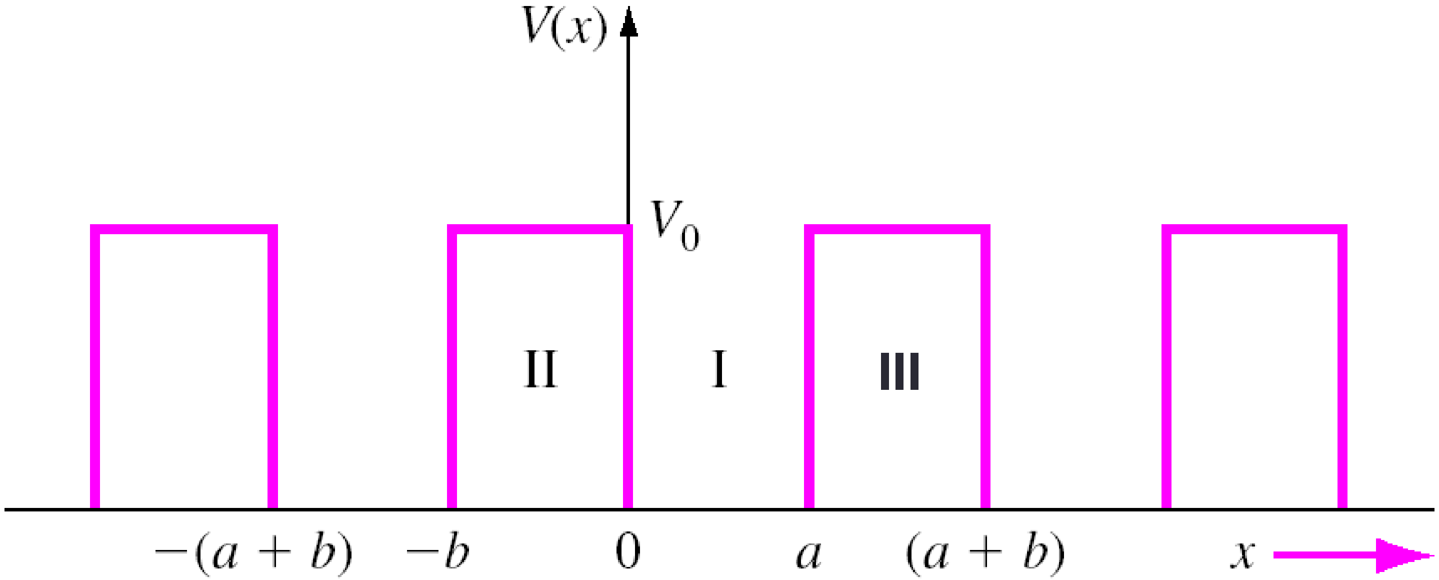
‡ Bloch, ' Z. Physik,' vol. 53, p. 216 (1929).

§ Peierls, ' Z. Physik,' vol. 53, p. 255 (1929).

‖ Kronig, ' Proc. Roy. Soc.,' A, vol. 124, p. 409 (1929).

Kronig – Penney model

- We approximate the periodic potential by a simpler model.



Kronig – Penney model

- Periodic potential⇔ Bloch waves as solutions
- The functions(and the derivatives) only differ by a factor of phase in region II and III

$$\varphi_{III}(x) = \varphi_{II}(x - a)e^{ika}$$

- Bound electrons in crystal⇔ $E<V_0$
- Potential $V(x)$ exists everywhere (everywhere finite) ⇔ wave function and its derivative have to be continue everywhere.

Kronig – Penney model

- Solving the Schrödinger’ Equation:
  - Region I (the well):

$$\varphi_I(x) = Ae^{i\beta x} + Be^{-i\beta x} \text{ avec } \beta = \sqrt{\frac{2mE}{\hbar^2}}$$

  - Region II (the barrier):

$$\varphi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x} \text{ avec } \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

  - Continuity of the wave function (and its first derivative) at *a* and -*b*: *be carreful of the phase shift at -b*

Kronig – Penney model

- We get now four homogeneous equations (2 for the wave function continuity and 2 for the first derivative continuity) with 4 unknows (A,B, C et D)

- Nontrivial solution (ie A=B=C=D=0) *if and only if* the determinant of the coefficients is zero

- We get (laborious, tedious but feasable !!)

$$\cos k(a+b) = \frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\beta a)\sinh(\alpha b)+\cos(\beta a)\cosh(\alpha b)$$

Reminder !! : k is a pseudo wave vector (crystal vector)!!

Kronig – Penney model

- And now ?

$$\cos k(a+b) = \frac{\alpha^2 - \beta^2}{2\alpha\beta}\sin(\beta a)\sinh(\alpha b) + \cos(\beta a)\cosh(\alpha b)$$

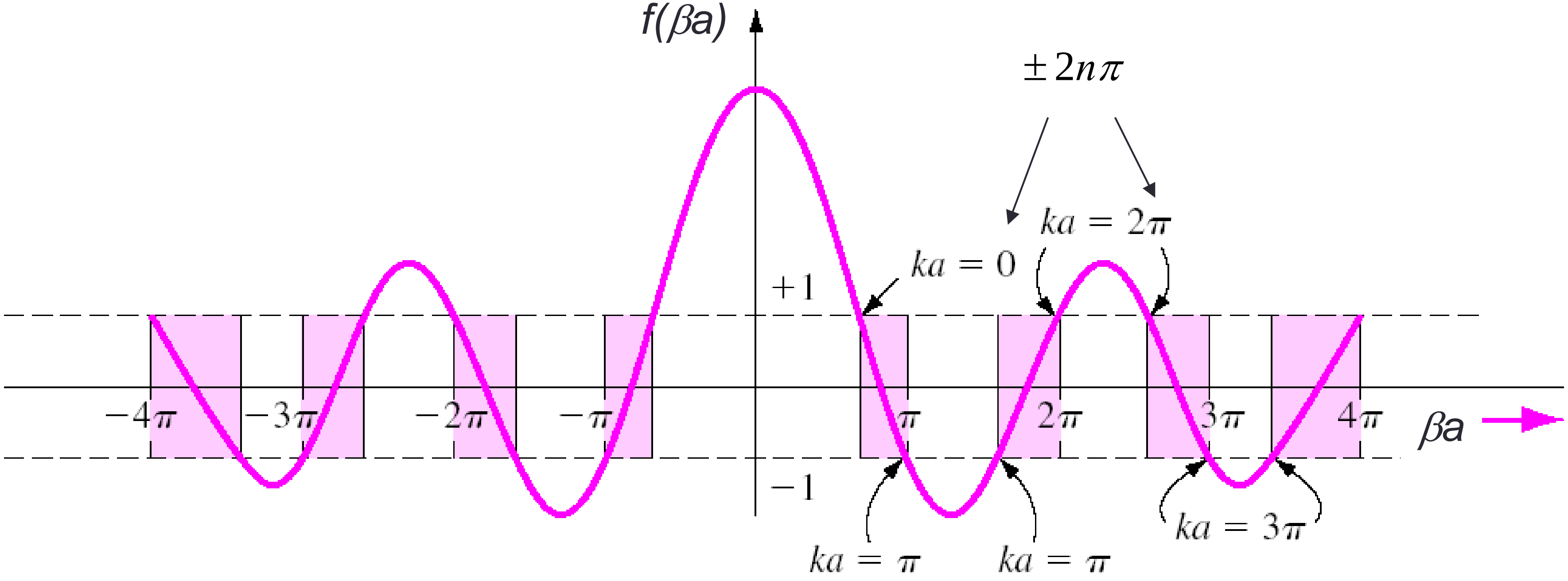
  - Graphics or digital solving to obtain a relation between *E, V_0* and *k*.
  - To be more realistics and to get more easely a « visible » graphics solution, let the potential barrier width b=>0 and the barrier height V_0=>∞ but with the product bxV_0 which remains finite

$$P\frac{\sin \beta a}{\beta a} + \cos \beta a = \cos ka \;\; \text{avec } P = \frac{mV_0 ba}{\hbar^2}$$

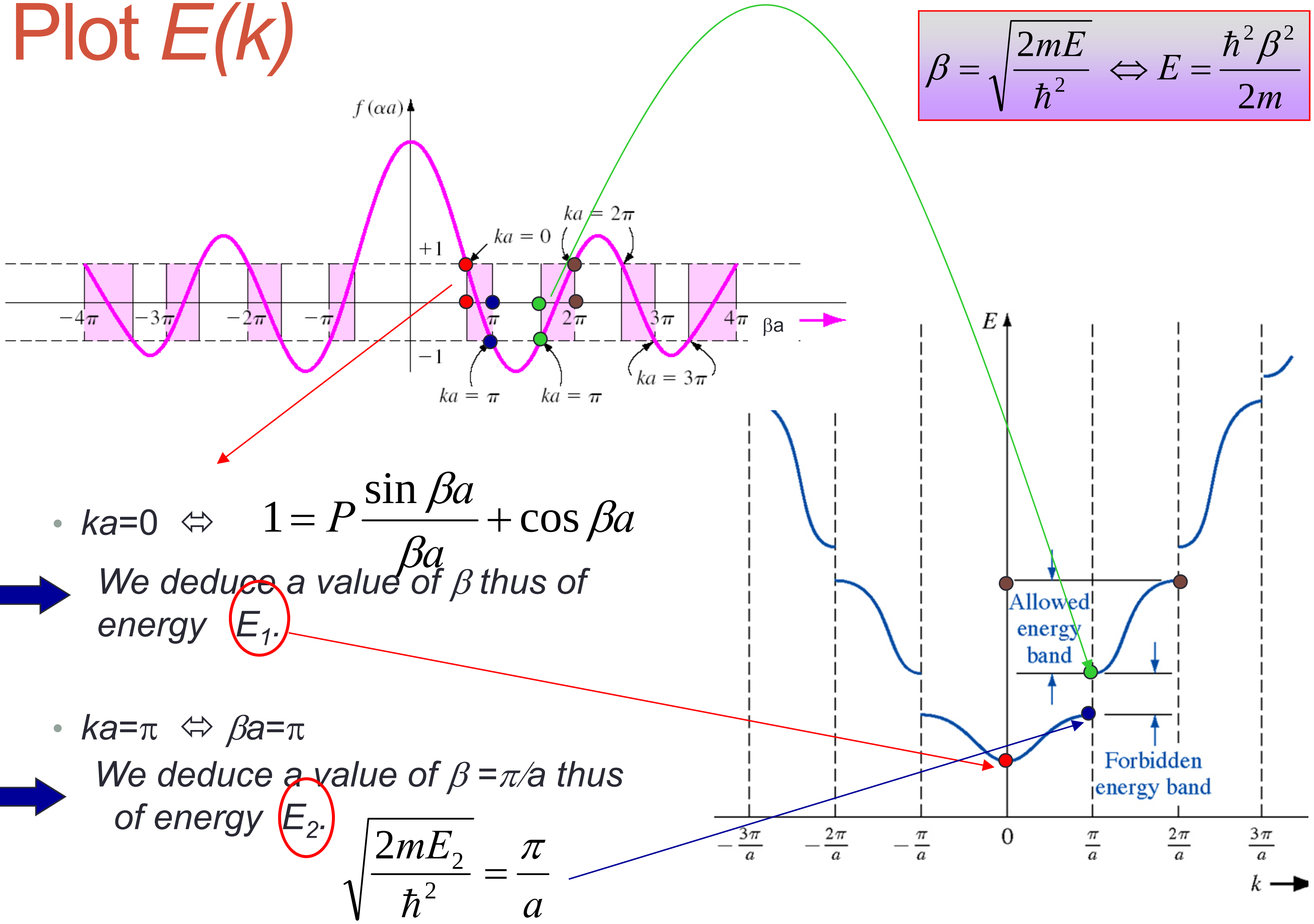
Kronig – Penney model

- Plot *E(k)*

$$P\frac{\sin \beta a}{\beta a}+\cos \beta a = f(\beta a) = \cos(ka)$$



Plot *E(k)*



$$\beta=\sqrt{\frac{2mE}{\hbar^2}} \Leftrightarrow E=\frac{\hbar^2\beta^2}{2m}$$

- *ka*=0 ⇔ $1=P\dfrac{\sin\beta a}{\beta a}+\cos\beta a$

We deduce a value of β *thus of energy* E_1.

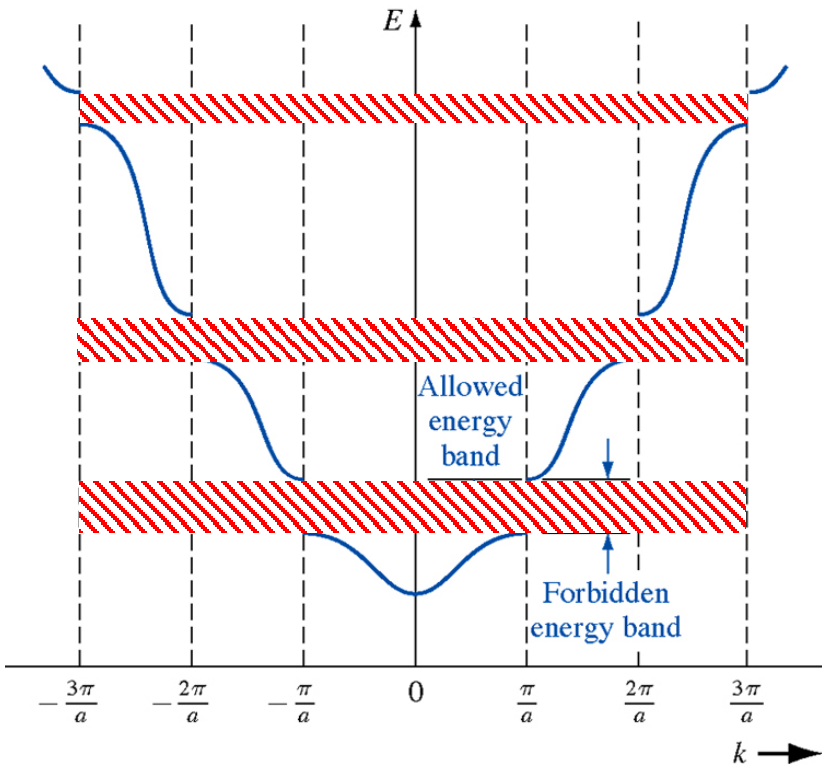
- *ka*=π ⇔ $\beta a=\pi$

We deduce a value of $\beta=\pi/a$ *thus of energy* E_2.

$$\sqrt{\frac{2mE_2}{\hbar^2}}=\frac{\pi}{a}$$

Energy bands

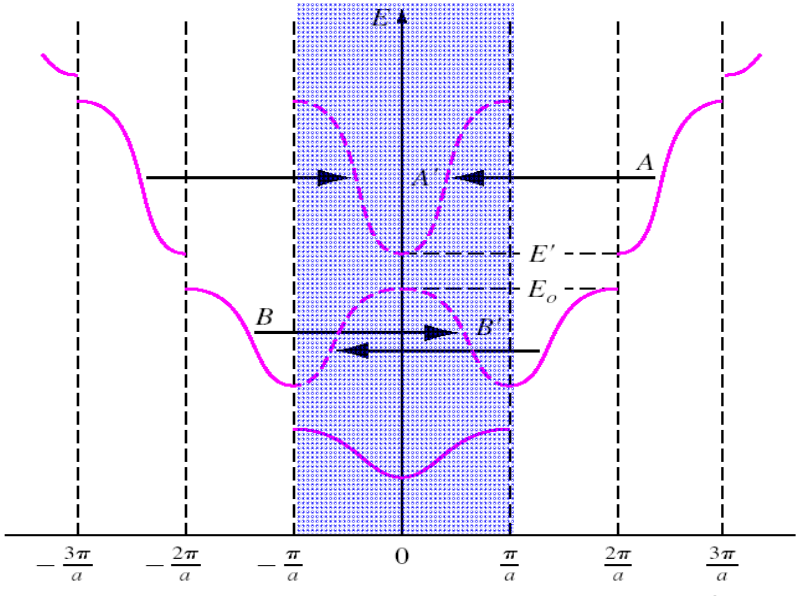
- As the partcle is propagating in a periodic potential (crystal potential), we have to introduce the notion/concept of allowed energy bands, separated to each other by forbidden energy band (▨) where we can not find particles.



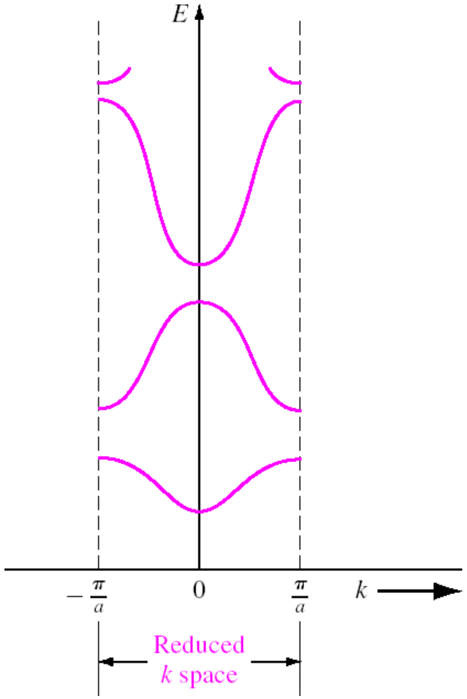
- Particles (electrons) are localised in allowed energy band
- As energy increases, the width of the allowed energy band increases
- We can plot E(k) only in a reduced zone *k:*
  - *$2n\pi$ periodicity*

$$\cos ka = \cos(ka + 2n\pi) = \cos(ka - 2n\pi)$$

Reduced zone representation



(From Neaman)



Concept of direct band gap : when the minimum of the upper band and the maximum of the lower band are localised on the same k value, we speak about direct band gap. This arrive in the center of zone (k=0) and in the edge zone ($k=\pm\pi/a$). Remind: this model is a 1D model, so a simpler model than the real model, but it's enough to introduce the energy band concept.

E(k) near an extremum

- Curve Sketching $\left.\frac{dE}{dk}\right|_{0,\pm\frac{\pi}{a}}$?
- E and k are not directly related!

$$\frac{dE}{dk} = \frac{dE}{d\beta}\frac{d\beta}{dk}$$

???

but

$$P\frac{\sin\beta a}{\beta a} + \cos\beta a = \cos ka$$

OK !

$$\frac{d[\cos ka]}{d\beta} = \frac{d[\cos ka]}{dk}\frac{dk}{d\beta} = \frac{d[P\frac{\sin\beta a}{\beta a} + \cos\beta a]}{d\beta}$$

We can show taht at center and at the edge of Brillouin zone,

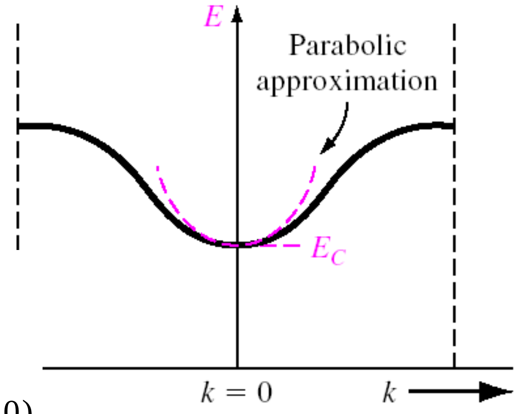
$$\boxed{\left.\frac{dE}{dk}\right|_{0,\pm\frac{\pi}{a}} = 0}$$

Effective mass

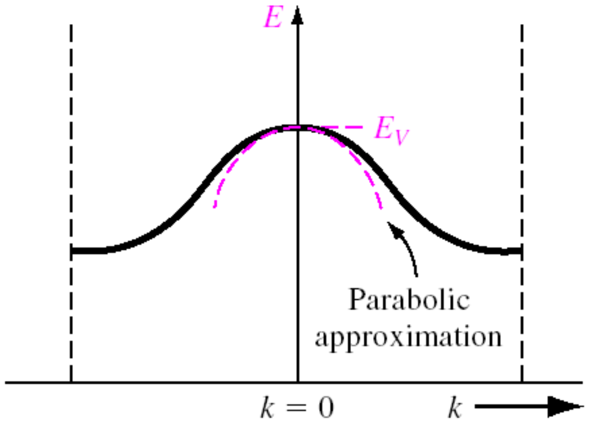
- Near the bottom (or top) of an extremum: (Taylor’s serie , second order)

$$E_k = E(0) + \underbrace{\left.\frac{dE}{dk}\right|_{k=0}}_{=0}(k-0) + \frac{1}{2!}\left.\frac{d^2E}{dk^2}\right|_{k=0}(k-0)^2$$

$$E_k = E_{(0)} + \frac{1}{2}\left.\frac{d^2E}{dk^2}\right|_{k=0} k^2 = E_{(0)} + \frac{\hbar^2 k^2}{2m^*} \text{ with } \frac{1}{m^*} = \frac{1}{\hbar^2}\left.\frac{d^2E}{dk^2}\right|_{(0)}$$



Within a certain range around the band extrema, we have the right to confuse the true curve with a parable: it is the approximation of the effective mass



Effective mass

- The effective mass is a parameter that relates the quantum mechanical results to the classical results).

- the idea is that when an electron is moving in a non constant potential (ie periodic potential) its inertia is modified and for continue to use the « classical » concept, we have to use this modified mass:

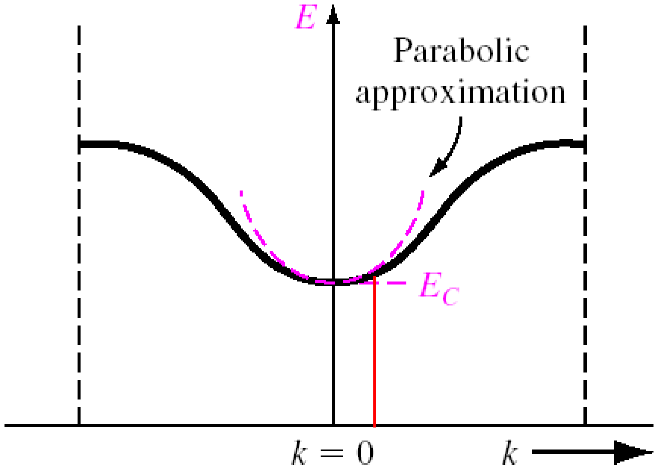
$$\boxed{\frac{dv_g}{dt} = \gamma = \frac{F}{m^*} \quad \text{avec} \quad \frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)_{k_0}}$$

Sign of the effective mass

- *Bottom :*

$$E_k = E_{(0)} + \frac{\hbar^2 k^2}{2m_1^*}$$

- $E_k > E_{(0)} = E_{minimum}$

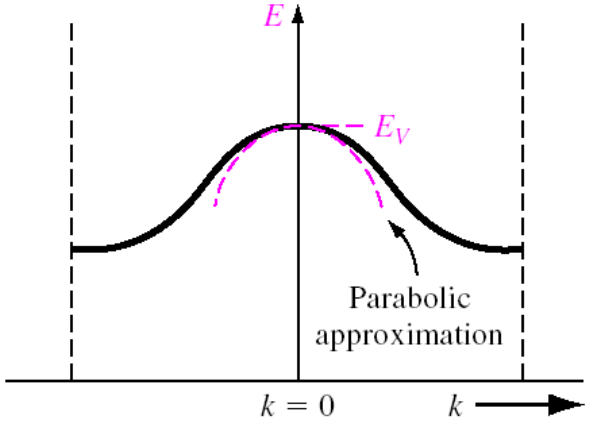


1st rule: the effective mass at the bottom band is a positive parameter

- *top:*

$$E_k = E_{Max} + \frac{\hbar^2 k^2}{2m_2^*}$$

2nd rule: the effective mass at the top band is a negative parameter



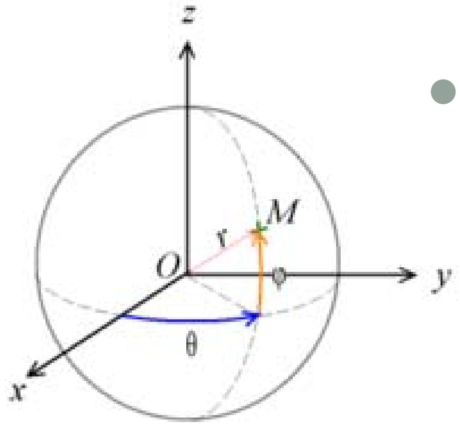
Density of states (mass effective approximation

- current⇔charges moving
- Need to count the number of charges in the bands (conduction or valence)
- This number is a function of allowed energy states in the bands
- Warning: we have to take into account Pauli exclusion principle

Density of states (mass effective approximation)

- Before continuing:
  - Concept of electron spin:

$$\varphi(r,\theta,\phi) = R(r).\Theta(\theta).\Phi(\phi)$$



- In addition to the three quantum numbers (principal, magnetic and azimuthal), the electron has an additional property which results by an intrinsic angular quantized momentum (± ½) to which is attributed a fourth quantum spin number, *s*, independent of the other 3.
- Principe d'exclusion de Pauli (dans les solides): we can not find two electrons in the solid with the same energy state (same quantum numbers).

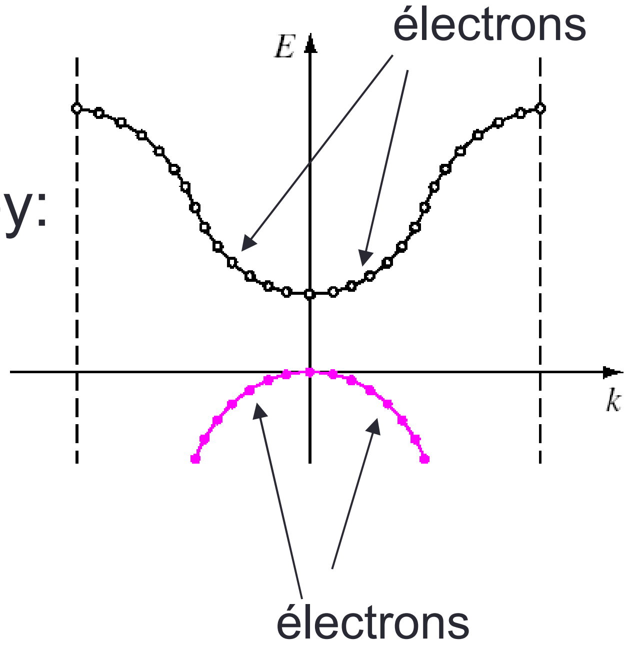
Density of states (mass effective approximation)

- Unidimensional crystal with a length L:

- allowed states are quantized and separated by $\Delta k = \dfrac{2\pi}{L}$
- near the minimum, on approxime E(k) by:

$$E = E_{\min} + \frac{\hbar^2 k^2}{2m^*}$$

- The quantum states density is the number of modes (states, places) per unit of energy and by unit length (L=1!):



$$g_{1D}(E) = \frac{dN}{dE} = \frac{\sqrt{2m^*}}{\pi\hbar}(E - E_{\min})^{-1/2} \quad J^{-1}m^{-1}$$

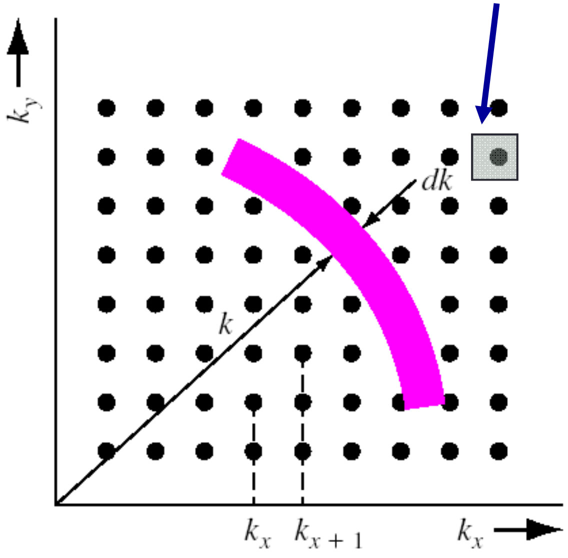
Density of states (mass effective approximation)

- Crystal 2D of dimensions L_x et L_y:

- Allowed states are allways quantized.
- Energy at the edge of the band (conduction or valence) is approximated by:

$$E = E_{\min} + \frac{\hbar^2 k^2}{2m^*}$$

« Surface » of an elementary state $\frac{(2\pi)^2}{L_x L_y}$



- The 2D states density is now given by:

$$\boxed{g_{2D}(E) = \frac{dN}{dE} = L_x L_y \frac{m^*}{\pi\hbar^2} J^{-1} \quad \text{ou} \quad \frac{m^*}{\pi\hbar^2} J^{-1} m^{-2}} \Bigg\}$$

No Energy dependent!

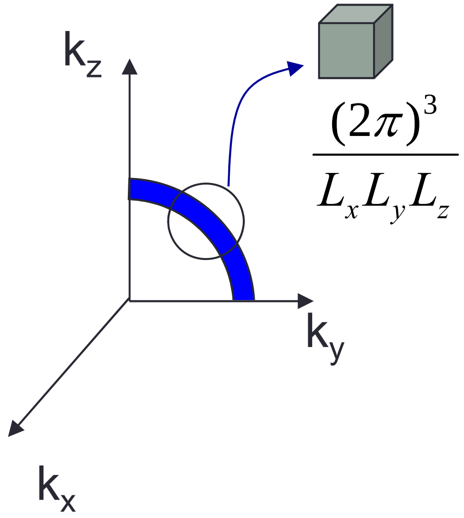
Density of states (mass effective approximation)

- 3D crystal with L_x, L_y and L_z for the dimensions:

- Allowed states are still quantized.
- Energy on top and bottom is given by:

$$E_{\vec{k}} = E_{\min} + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2) = E_{\min} + \frac{\hbar^2 \vec{k}^2}{2m^*}$$

- The density of states is given by (with *L_x x L_y x L_z=1* ie per volume):



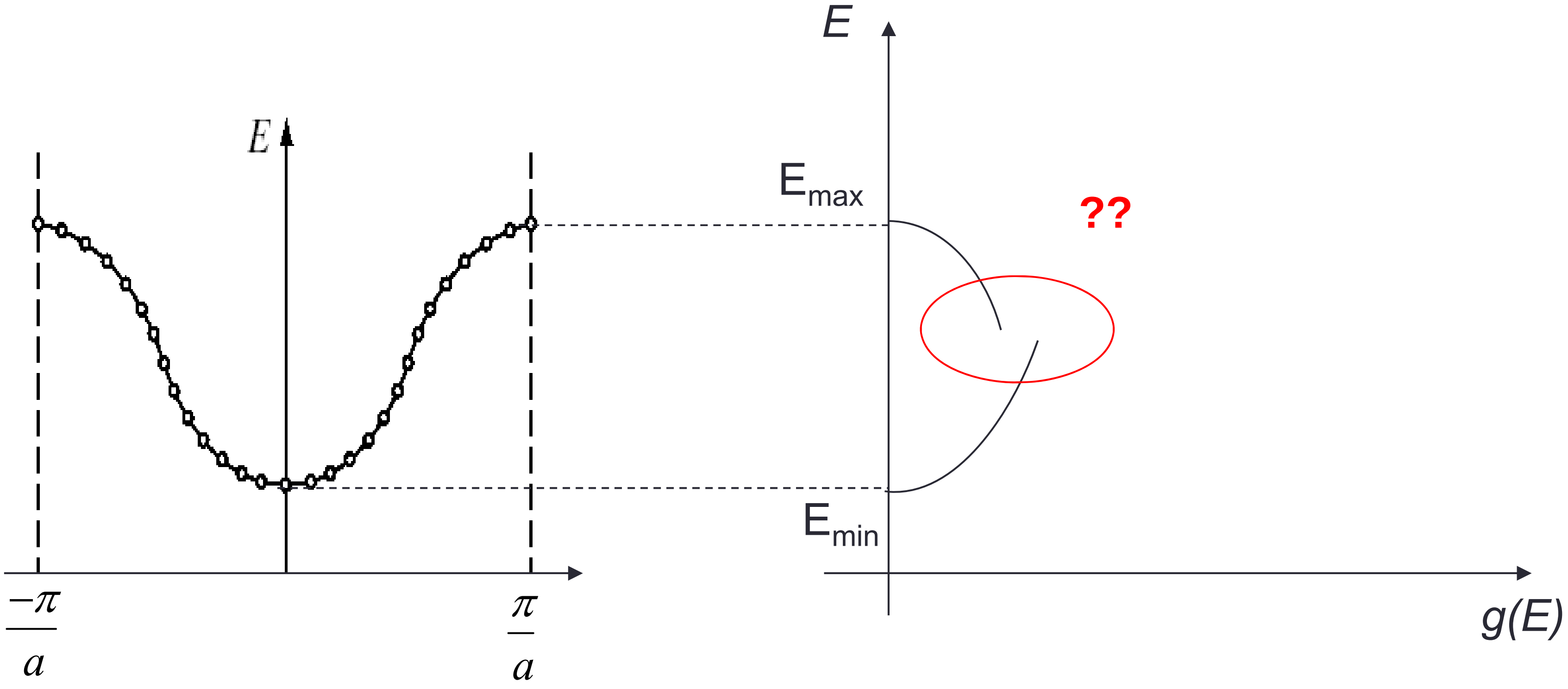
$$g_{3D}(E) = \frac{dN}{dE} = 4\pi\left(\frac{2m^*}{h^2}\right)^{3/2}(E - E_{\min})^{1/2} J^{-1} m^{-3} \longleftarrow$$

bottom

$$\underline{\qquad\quad} = \underline{\qquad\qquad\qquad\qquad} (E_{\max} - E)^{1/2} \longleftarrow$$

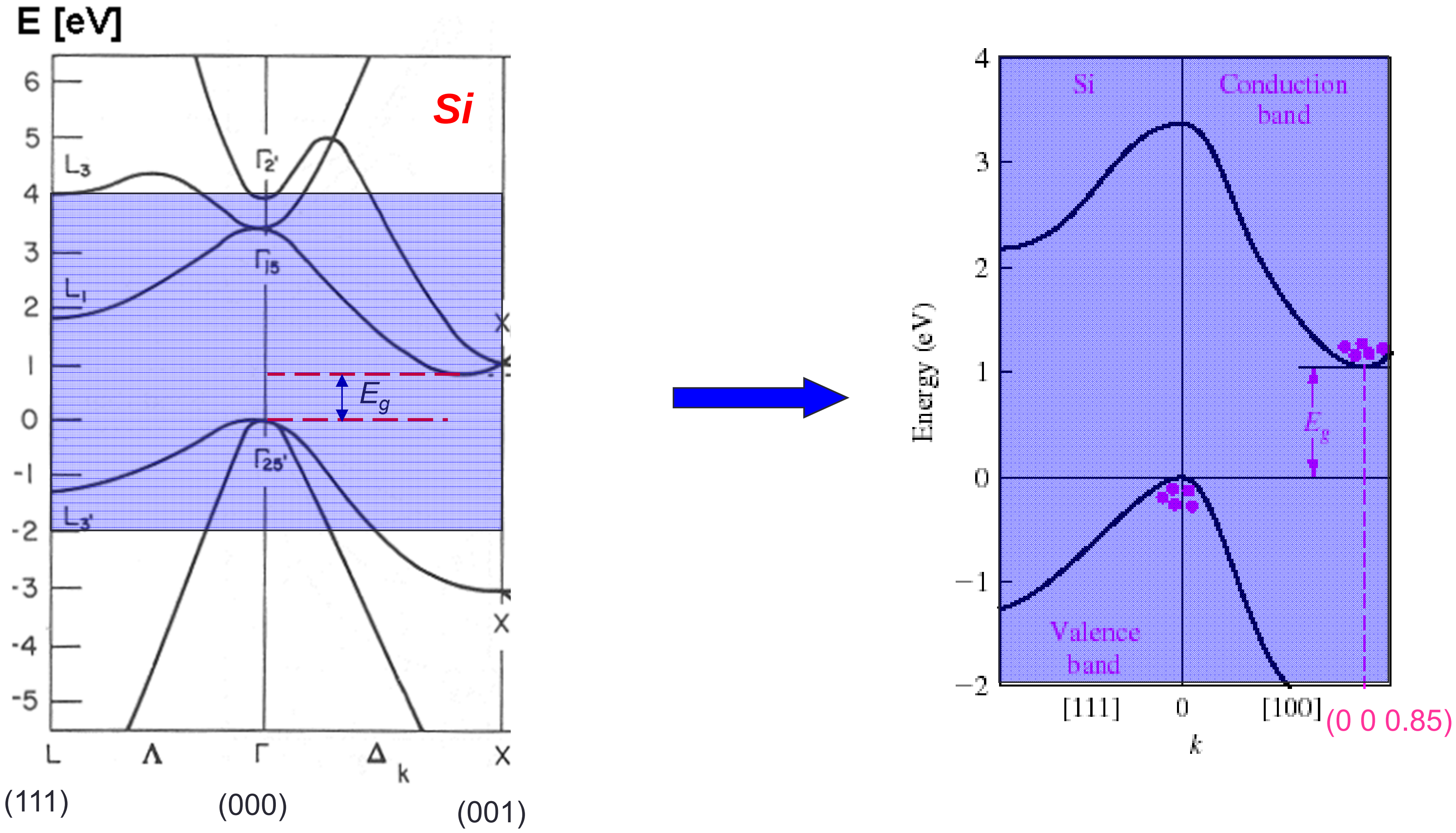
top

3D states density

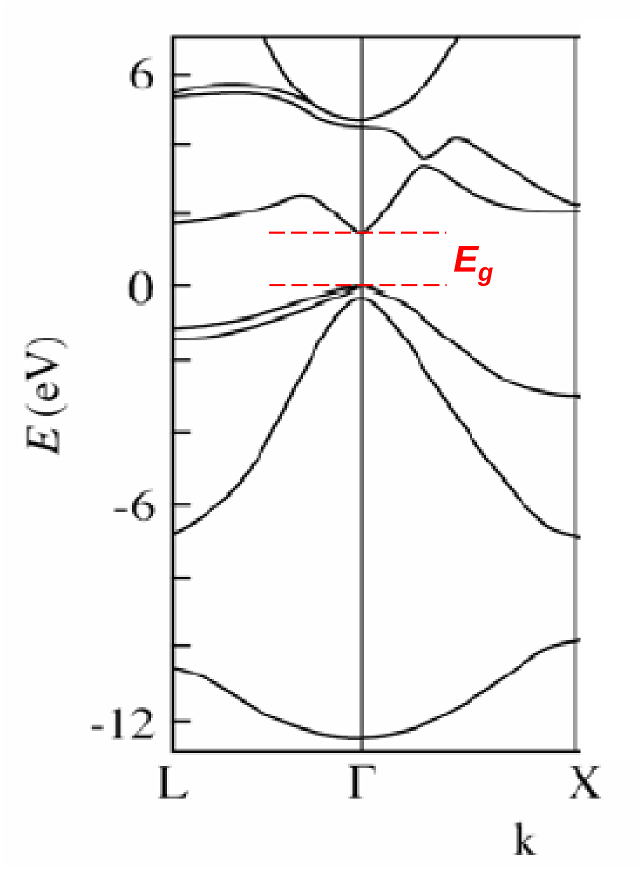


*The effective masses are not the same and the approximation of m * only applies on band edge!*

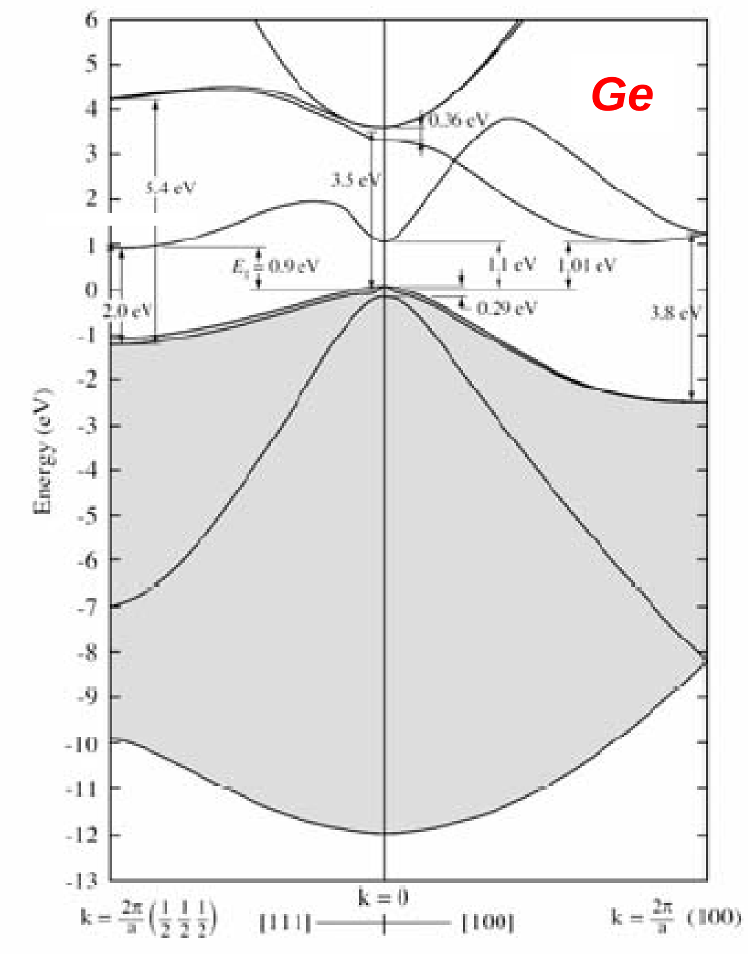
Real crystal band structure!



Real crystal band structure!



GaAs



synthesis

- Crystal ⇔ periodic potential
  - introduction of energy band concept
  - Introduction of forbidden energy band

Is it enough to explain the difference between metal and insulator (or semiconductor)?
To be continued in the next chapter

CHAPITRE 7

Current in the solids:
Specific case of semiconductors

Conduction current in the Bloch – Brillouin crystal

- Density of current vector:
  - Current density ? It's a moving of electric charges per time and per surface

$$\vec{j} = -q\sum_i n_i \vec{v_i} = -q\sum_i \vec{v_i}$$

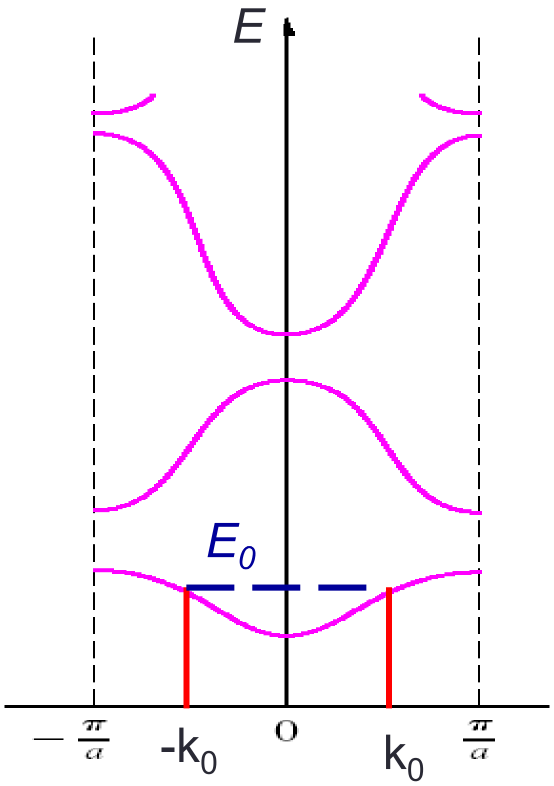
with n_i number (1D density) of electrons with velocity $\vec{v_i}$

  - At 1 dim:

$$\overline{j} = -q\sum_i \overline{v_i}$$

Conduction current in the Bloch – Brillouin crystal

- Contribution of the various bands to electric current
- *Full band*



- On each allowed values of k_0 we can form a wave packet
- The band is full if all allowed states of k_0 are occupied (all energy levels are occupied).
- E(k) is even with k ⇔ $E(-k_0)= E(+k_0)$ ⇔ the probability of find the electron at k_0 or at $-k_0$ is the same (see next chapter)
- The velocity $v_g = \frac{1}{\hbar}\left(\frac{dE}{dk}\right)_{k_0}$ of the particle is odd with k ⇔ $v_g(k)=-v_g(-k)$

$$\boxed{\overline{j} = -q\sum_i \overline{v_i} = 0 \quad \text{(the band is full)}}$$

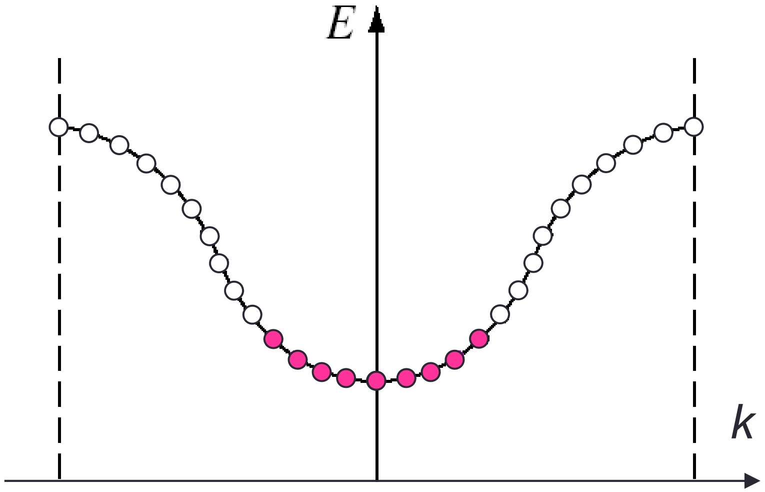
Conduction current in the Bloch – Brillouin crystal

- *Rule 1*: the contribution to the current for a full band is allways zero.
- *Rule 2*: the contribution to the current for an empty band is of course zero.
- *Corollary* : the electric current in only due to partially filled band

Contibution with a partially filled band

- Perfect crystal, $\mathcal{E}_{elec}$ = 0 and uniform Temperature.
  - Thermodynamical equilibrium
  - Occupancy probabilities of the energy states k and -k are identical

$$\boxed{\overline{j} = -q\sum_i \overline{v_i} = 0 \qquad [v_g(k) = -v_g(-k)]}$$

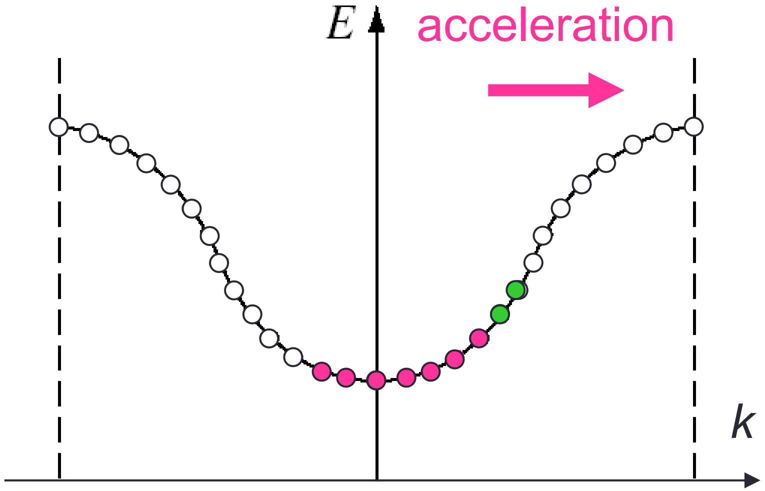


- Not surprising results : no electric field ⇔ no conduction current!

Contribution with a partially filled band

- Perfect crystal, $\mathcal{E}_{elec} \neq 0$ and uniform Temperature.
  - At time = 0, we apply an electric field $\mathcal{E}_{elec}$.
  - A wave packet (in fact an electron) wich « had » before k_0 undergoes an acceleration

$$\hbar \frac{dk_0}{dt} = -q\overline{\varepsilon_{elec}}$$



  - At time >0,

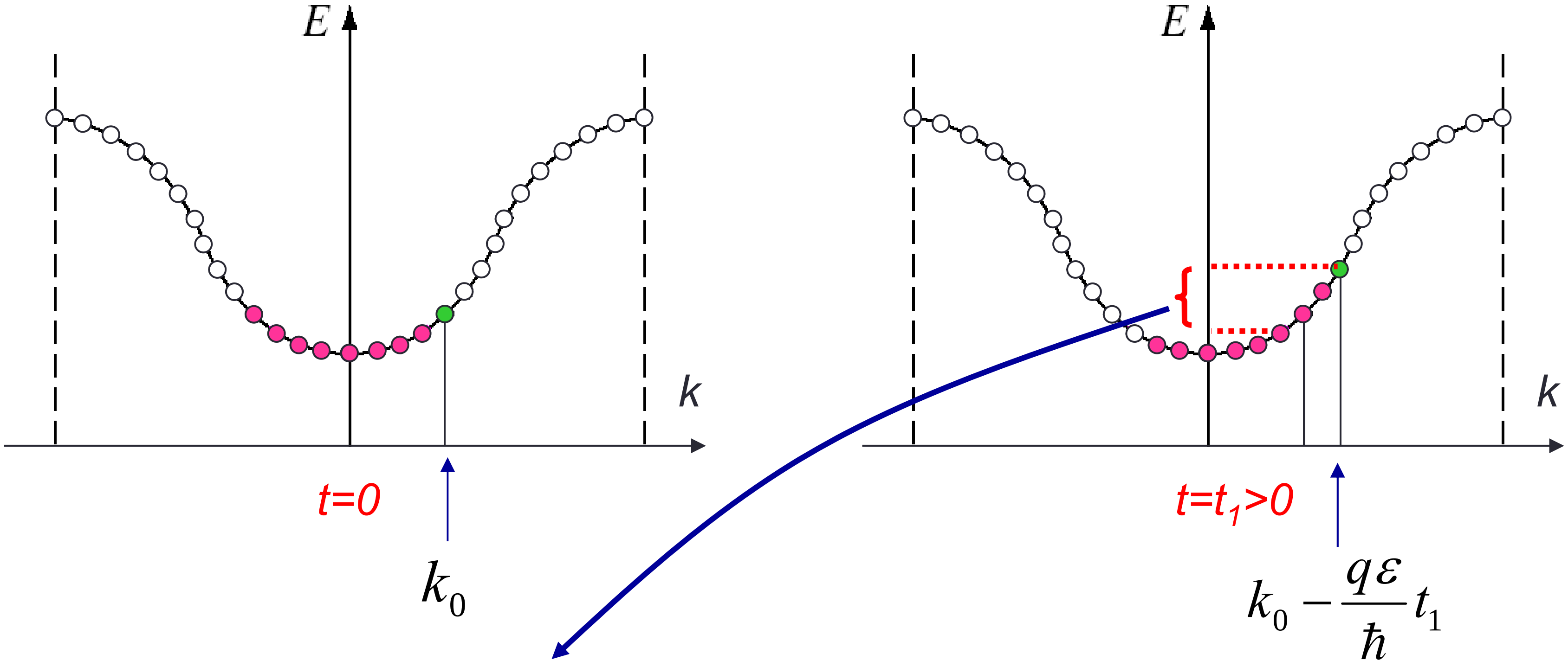
$$k_0^{'}(t) = k_0 - q\frac{\overline{\varepsilon}}{\hbar}t$$

  - All electrons undergo the same variation Δk

$$\Delta\overline{k_0} = -q\times\frac{\varepsilon}{\hbar}\times t \quad \forall\overline{k_0}$$

Contribution with a partially filled band

- Perfect crystal, $\mathcal{E}_{elec} \neq 0$ and uniform Temperature.

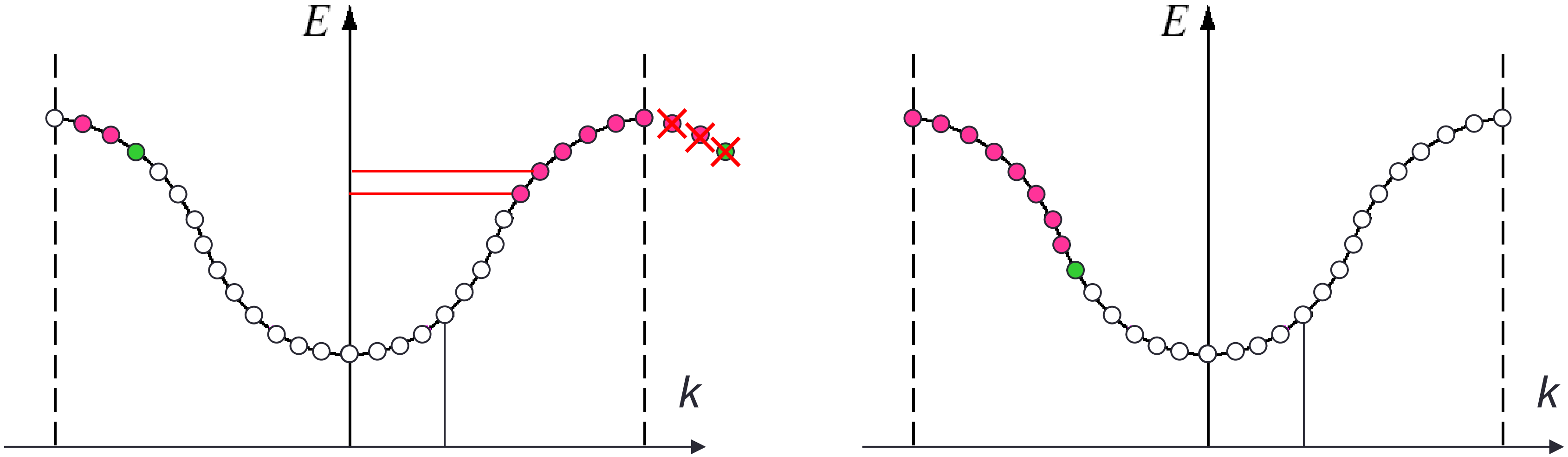


Now all velocities are not balaced/compensated!

$$\Rightarrow \quad J(t_1) \neq 0 > 0$$

Contribution with a partially filled band

- Perfect crystal, $\mathcal{E}_{elec} \neq 0$ and uniform temperature.



$t_2 > t_1$

$t_3 > t_2$

$$J(t_2) \neq 0 > 0$$

$$J(t_3) \neq 0 < 0 \quad !!!$$

Strange ! Electric field is constant and current is alternatively changing (its sign), function of the time !!

Contribution with a partially filled band

- in the Bloch – Brillouin model, we predict that a constant applied field ε_{elec} must generate an alternative electric current .
- La période de ce courant serait:

$$\hbar \frac{dk}{dt} = -q\varepsilon \quad \Rightarrow \quad \hbar \frac{2\pi}{a}\frac{1}{T} = -q\bar{\varepsilon} \quad \Rightarrow \quad \boxed{T = \frac{\hbar \, {}^{2\pi}\!/\!_{a}}{q\bar{\varepsilon}}}$$

- This result is not coherent with experimental results !!!!

- The crystal is not as perfect as it!!

The real crystal in the Bloch-Brillouin model

- Real crystal, $\varepsilon_{elec} \neq 0$ and uniform Temperature.
  - The crystal has a number of defects ⇔ main class:
    - Chemical impureties
    - Intrinsic point defects :
      - Vacancy
      - Interstitials
      - Antisites
    - Défauts étendus
      - Grain boudaries
      - Stacking defects
      - Dislocations
      - Clusters
    - Lattice vibration/oscillation around equilibrium position (phonons)

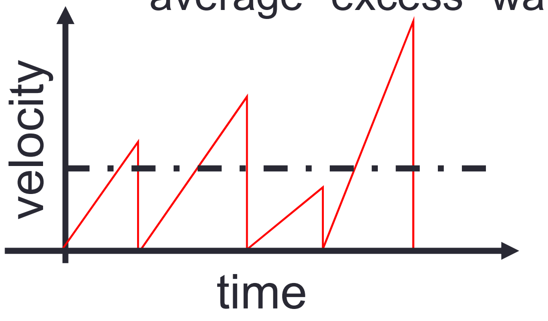
The real crystal in the Bloch-Brillouin model

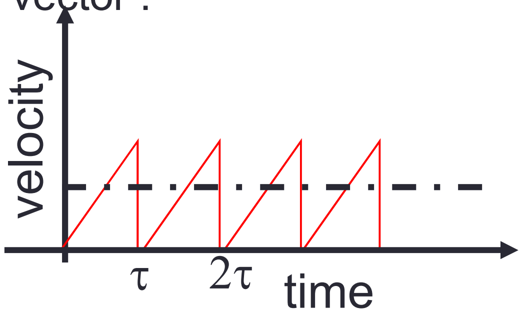
- Real crystal: consequence on charge carrier:
  - The BB potential is no more exactly periodic potential:
    - B-B $v_1(x)=v_1(x+a)$
    - *Réel* $v(x)=v_1(x)+\Delta v(x)$ → random!
  - Electron in this potential experiences a force (-gradv(x))

$$\boxed{\hbar\frac{dk_0}{dt} = -q\varepsilon - grad(\Delta V(x)) = -q\varepsilon + random\ \ force}$$

  - This force gives random pulse(similar to forces during impacts with « impureties »)

  - On average, every τ (average time between subsequent collisions), the electron changes direction and especially loses its kinetic energy ⇔ therefore acquires an average "excess" wave vector :

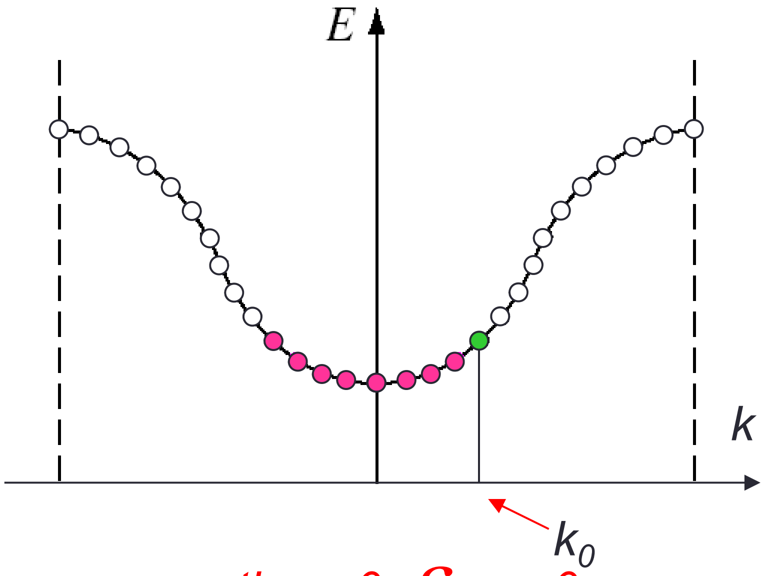




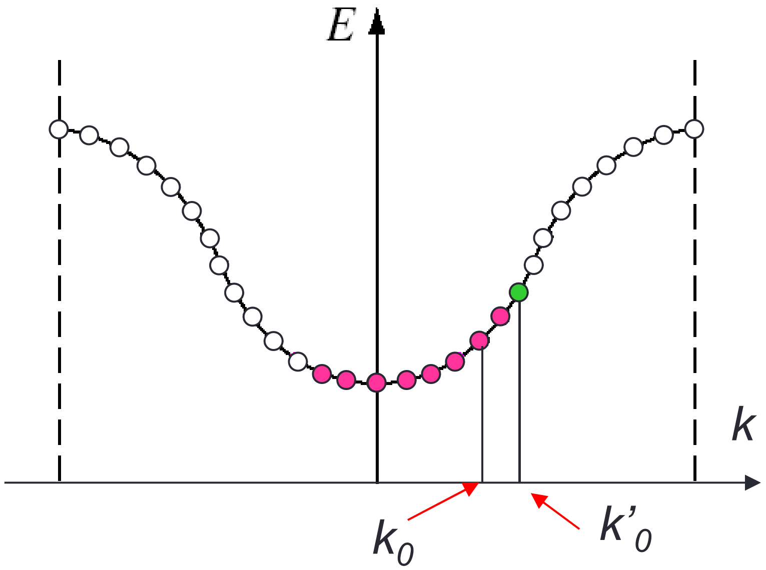
$$k_0' = k_0 - q\frac{\varepsilon}{\hbar}\tau \qquad \underline{\forall\, t}$$

The real crystal in the Bloch-Brillouin model

- Real crystal, $\mathcal{E}_{elec} \neq 0$ and uniform Temperature.



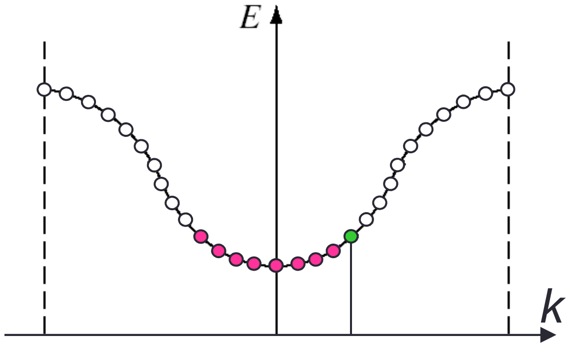
time=0, $\mathcal{E}_{elec}=0$



time≠0 , $\mathcal{E}_{elec}\neq 0$

$$k_0' = k_0 - q\frac{\varepsilon}{\hbar}\tau \qquad \underline{\forall\, t}$$

Real crystal in Bloch-Brillouin model



- *Almost empty band:*
  - Energy and group velocity:

- $\mathcal{E}=0$:

$$E_{k_0} = E_c + \frac{\hbar^2 k_0^2}{2m_1^*} \qquad v_g = \frac{1}{\hbar}\left(\frac{dE}{dk}\right)_{k_0} = \frac{\hbar}{m_1^*}k_0 \qquad k_0' = k_0 - q\frac{\varepsilon}{\hbar}\tau$$

$$\boxed{\overline{j} = -q\sum_i \overline{v_{g_i}} = -q\frac{\hbar}{m_1^*}\sum_i k_i = 0}$$

- $\mathcal{E}\neq 0$:

$$\boxed{\overline{j} = -q\sum_i \overline{v_{g_i}} = -q\frac{\hbar}{m_1^*}\sum_i k_i' = -q\cancel{\frac{\hbar}{m_1^*}\sum_i k_i} + q^2\frac{\hbar}{m_1^*}\frac{\varepsilon_{elec}\tau}{\hbar}n}$$

$$\overline{j} = q\mu_n n\varepsilon_{elec} \qquad \text{with } \mu_n = q\frac{\tau}{m_1^*} > 0$$

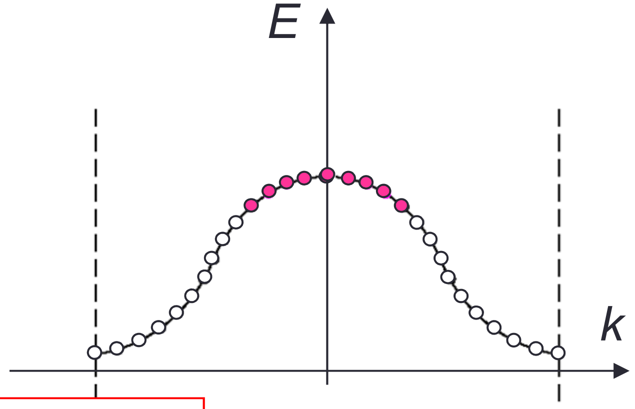
↑ Mobility (cm²/Vs)

$$\overline{j} = \sigma_n\varepsilon_{elec}$$

It's Ohm's law

Real crystal in Bloch-Brillouin model

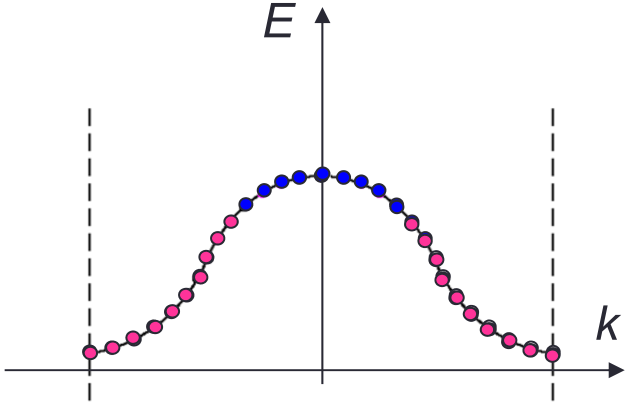
- *Almost full band:*
  - trick: to calculate the electric current in an almost full band, we add the missing electrons to fill the band and then we remove them: which will allow us to introduce the concept of holes.
    - N : number of places (~ number of atoms)
    - N-p: electrons on the band
    - p: empty places (states) or number of states



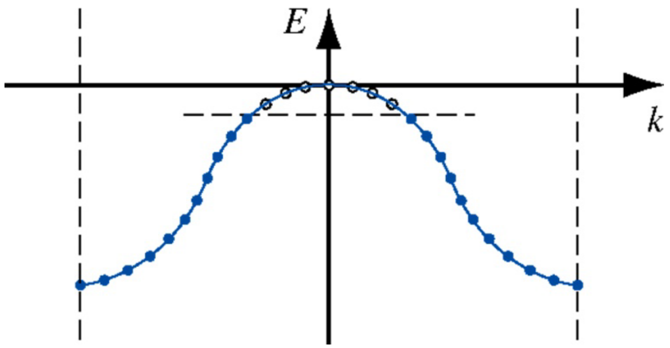
$$\boxed{\begin{aligned}\bar{j} &= -q\sum_{i=1}^{N-p} v_{g_i} = -q\sum_{i=1}^{N} v_{g_i} - \left(-q\sum_{i=1}^{p} v_{g_i}\right) \\ &= \underbrace{0}_{\text{Full band}} + q\sum_{i=1}^{p} v_{g_i}\end{aligned}}$$

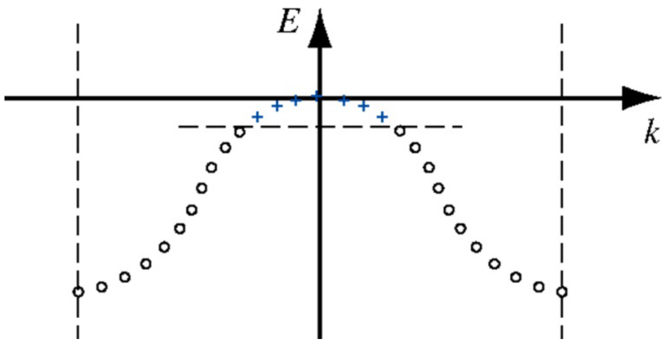
Positive charge!

Real crystal in Bloch-Brillouin model

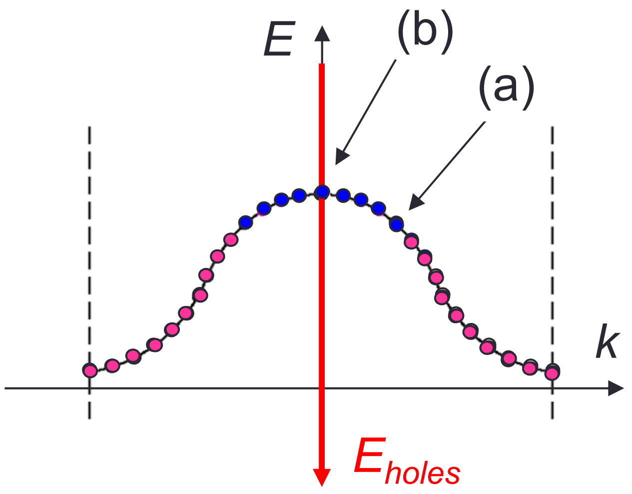


- *Almost full band:*
  - Rule: la contribution au courant d'une bande presque pleine est obtenue en supposant que les états vides sont effectivement occupés par des porteurs de charges positives +q: des trous. Il suffit de sommer sur le nombre total de trous
  - Trous: paquet d'ondes de charges positives





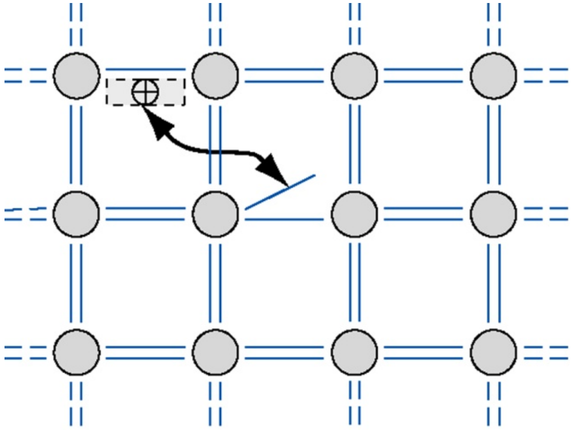
Concept of the Hole



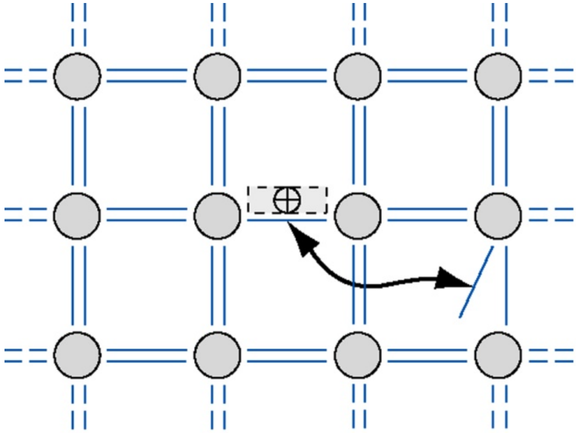
- Drift current:
  - Nota: to “extract" an electron in (a) requires more energy than (b)⬄ a hole in (a) is more energetic than in (b).
  - E(e⁻) = -E(h⁺) ⬄ $E_{holes} = -E_V + \frac{\hbar^2 k^2}{2m*} \Rightarrow v_g^{holes} = \frac{\hbar k_0}{m*}$
  - $\varepsilon_{elec}=0$ ⬄ $J = q\left[\frac{\hbar}{m*}\sum \overline{k_0}\right] = 0$
  - $\varepsilon_{elec}\neq 0$ ⬄ $J = q\left[\frac{\hbar}{m_2^*}\sum_{i=1}^{p}\left(\overline{k_0} + q\frac{\varepsilon_{elec}\tau}{\hbar}\right)\right] = \frac{q^2\hbar}{m_2^*}\frac{\varepsilon_{elec}}{\hbar}\tau \times p$

$$\boxed{J = q \times p \times \mu_p \times \varepsilon_{elec} \quad \text{with} \quad \mu_p = \frac{q\tau}{m_2^*}}$$

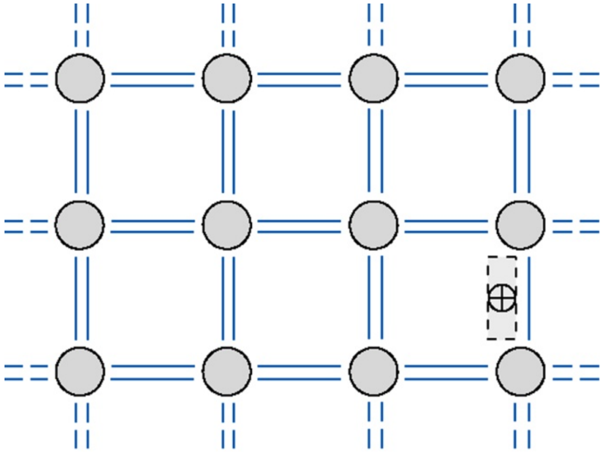
Concept of hole : conduction



(a)



(b)



(c)

Bipolar (electrons and holes) conduction

- Common case in semiconductors :
  - In practice, in the semiconductor, there is an almost empty band, called conduction band (CB), over a nearly full band called the valence band (VB). They are separated by a forbidden energy band ("gap or bandgap"). The current is the sum of the two components

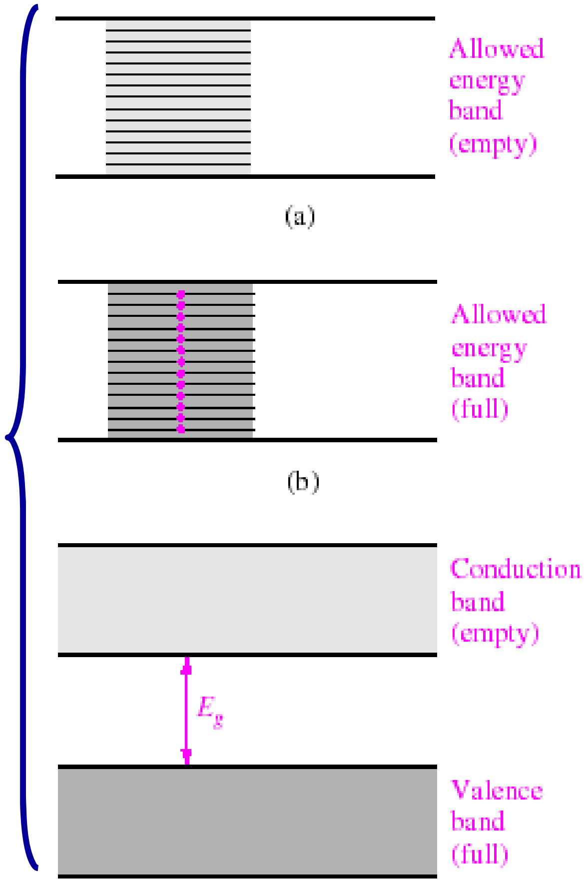
$$\overline{J} = \underbrace{qn\mu_n\varepsilon}_{BC} + \underbrace{qp\mu_p\varepsilon}_{BV} = \sigma\varepsilon$$

Semiconductor or insulator?

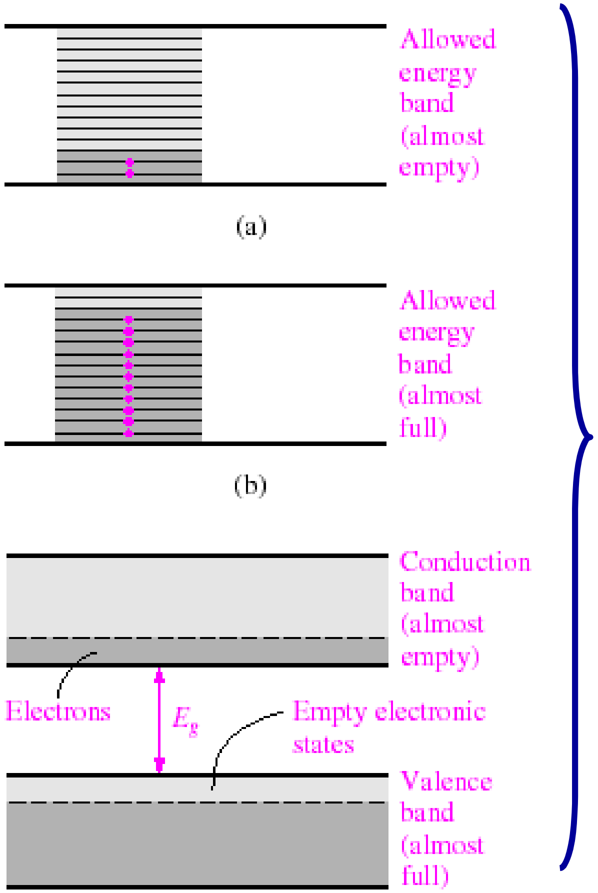
- Same energy band diagram? The only difference is the value of the bandgap. If Eg larger than 3.5/4 eV ⇔ insulator

T= 0 K

Isolant , semiconducteur



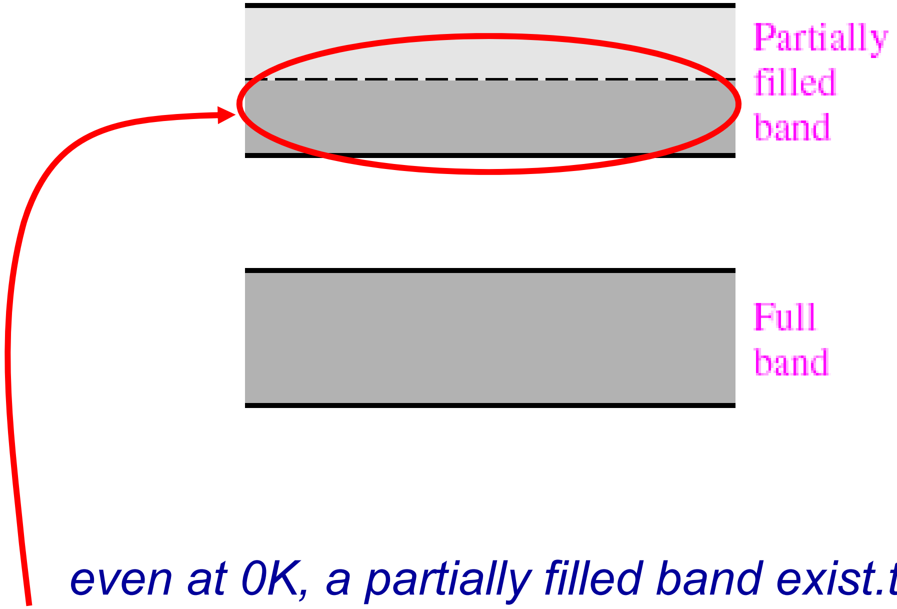
semiconducteur



T ≠ 0 K

Metal ?

- T=0K ou T≠ 0K



even at 0K, a partially filled band exist.this band conducts. An other way to get a metal is the existence of overllaping allowed energy bands (semi metal)

Summary:

- Metal:
  - Very low resistivity
  - When the temperature is lowering, the conductivity increases

- Insulator:
  - No conduction even at high temperature
  - Bandgap higher than 3.5 eV

- Semiconductor:
  - Bandgap lower than 3 eV
  - The conductivity is not a monotone function of the temperature.

CHAPTER 8

Statistical mechanics : Fermi – Dirac function and Maxwell – Boltzmann function

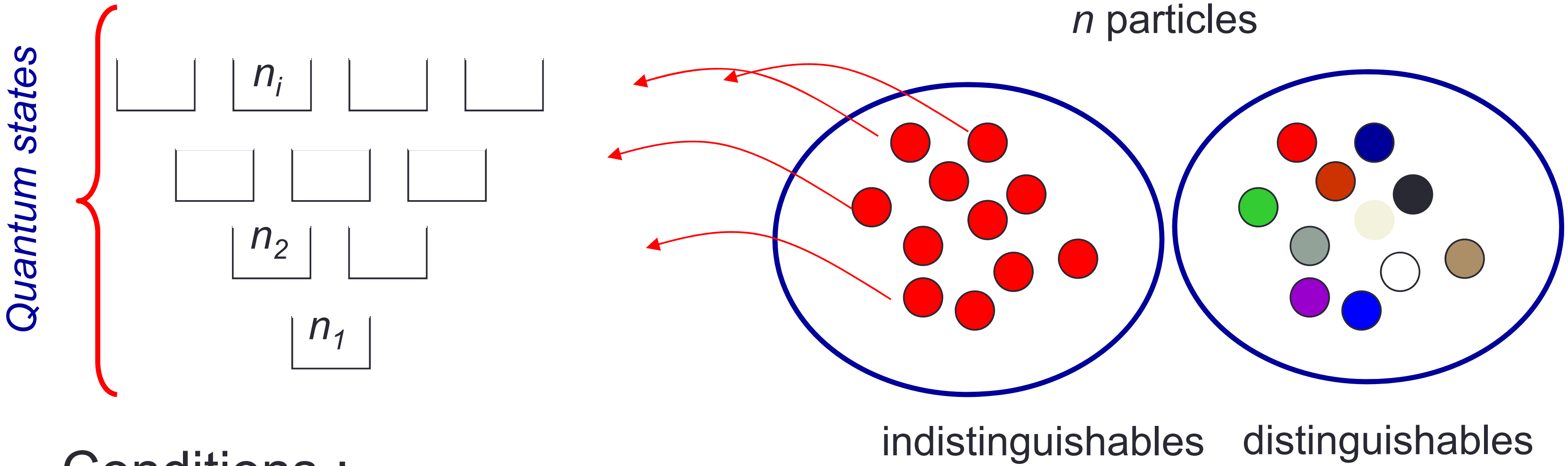
The statistics

- Maxwell – Boltzmann
  - Distinguishable particle
  - Gas molecules at fairly low pressure
- Bose – Einstein
  - Indistinguishable particle
  - Several particles permitted in each quantum state
    - Photons, Phonons
- Fermi – Dirac
  - Indistinguishable particle
  - Only one particule in each quantum state (Pauli principle
    - Electron in the crystal, solids

In each statistics, particles are assumed to be noninteracting

The statistics

- Solving methods:



- Conditions :
  - Number of particles is constant : $\sum_i n_i = n$
  - Internal energy is constant : $\sum_i n_i E_i = E$
  - Indistinguishables or distinguishables ?
  - One or more particles in each quantum state?

Maxwell – Boltzmann

- Distinguishable
- Each state can be occupied by unlimited number of particles
- Equilibrium state is the one which is the most probable

- Consider an equilibrium state with n_1 particules in c_1, n_2 in c_2, …. , n_i in c_i.
- What is the probability of this configuration?

$$P = \frac{n!}{n_1! n_2! \dots n_i! \dots} = \frac{n!}{\prod_i n_i!}$$

- This configuration is the equilibrium one if P or *ln*(P) is maximum⇔ d(lnP)=0
- We then get

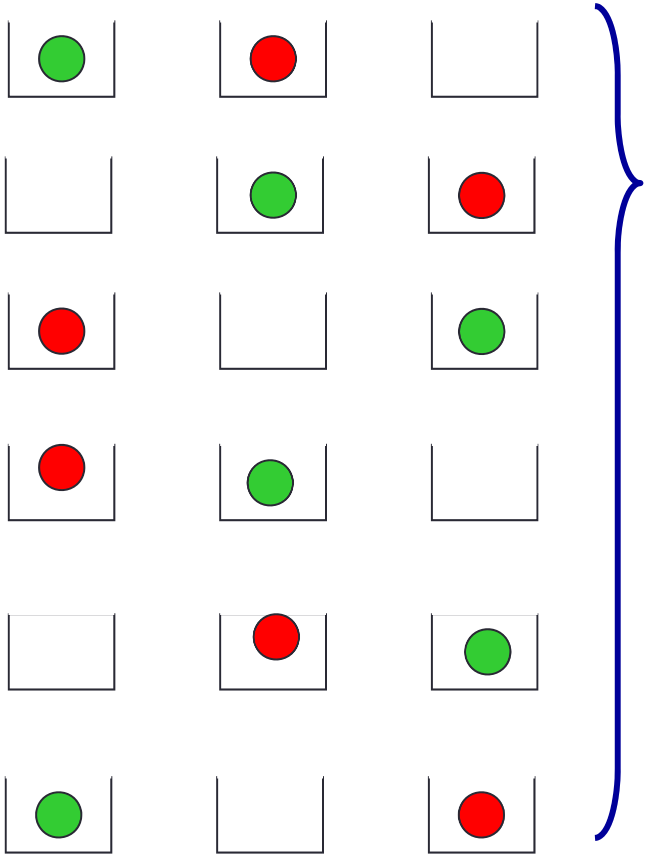
$$f(E_i) = \frac{n_i}{g_i} = e^{-(E_i - E_F)/kT}$$

n_i: number of particles in E_i
g_i : number of places (staes) on E_i

Distinguishable or not

(1 « ball » in each case ⇔ Pauli)

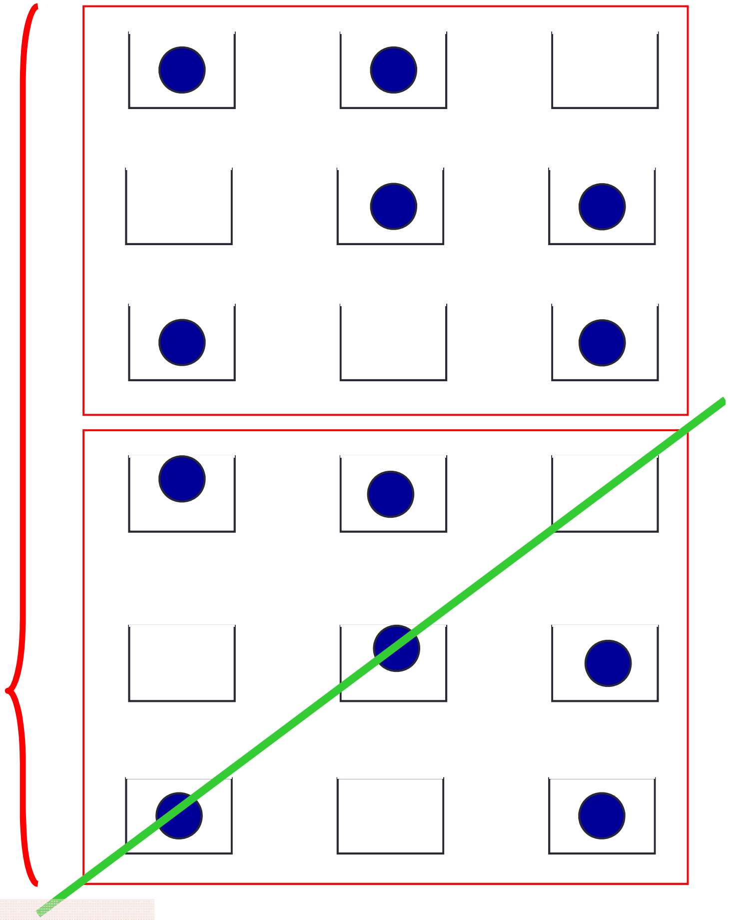
Distinguishable



$$\frac{g_i!}{(g_i - N_i)!}$$

$$\frac{g_i!}{\boxed{N_i!}(g_i - N_i)!}$$

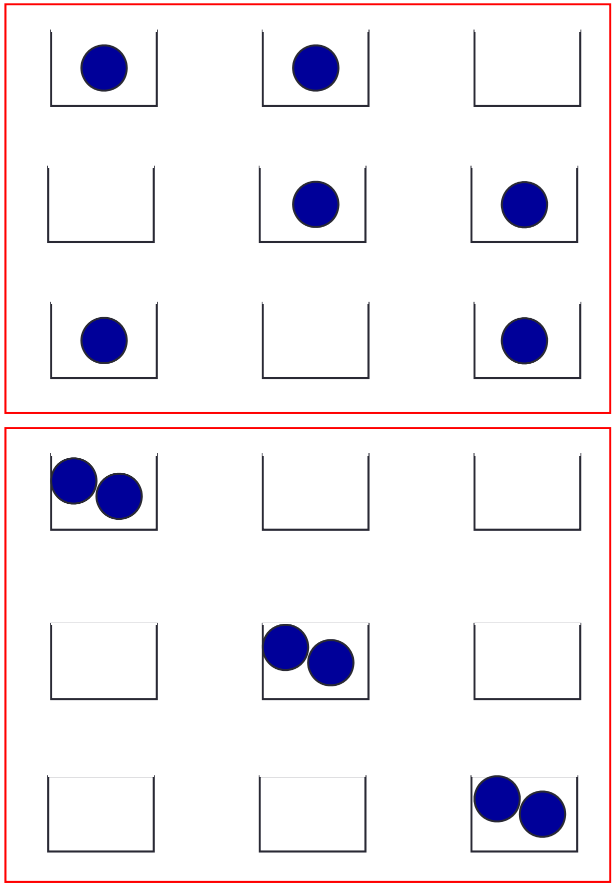
undistinguishable



n_i: number of particles in E_i
g_i : number of places (staes) on E_i

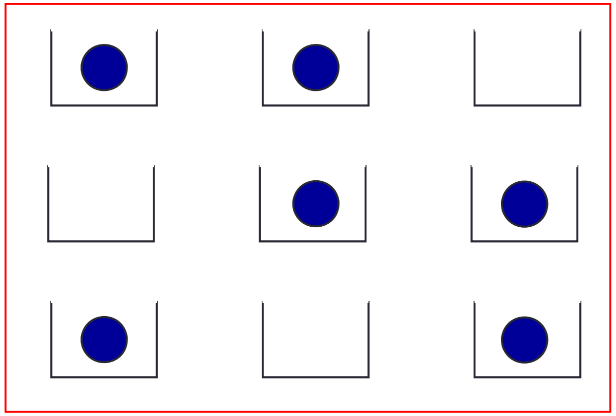
Undistinguishable

« Bose »



$$\frac{(N_i + g_i - 1)!}{(g_i - 1)!\,N_i!}$$

« Pauli »



$$\frac{g_i!}{N_i!(g_i - N_i)!}$$

n_i: number of particles in E_i
g_i : number of places (staes) on E_i

Fermi –Dirac statistics

- Same approach than before

$$\frac{g_i!}{N_i!(g_i - N_i)!}$$

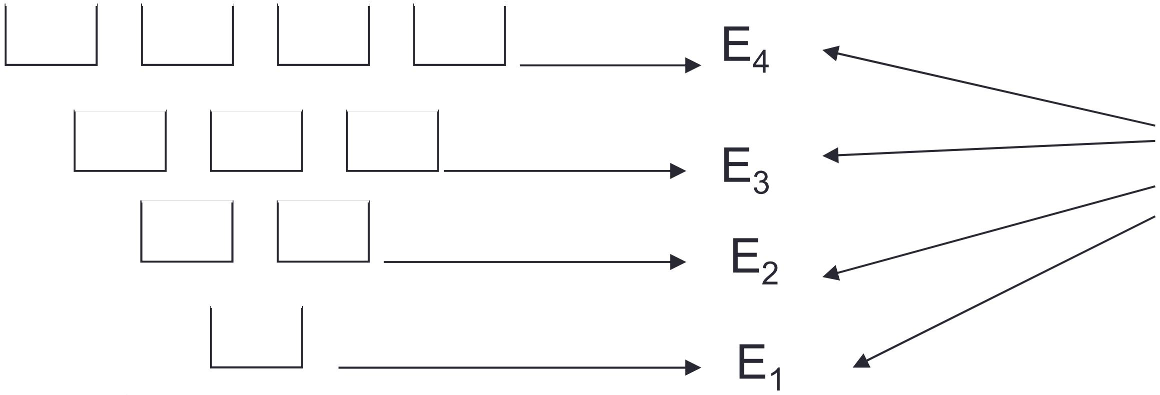
  - Energy level E_i, degenerated g_i times (it means g_i « boxes » or cells/ quantum states with the same energy E_i) and N_i particles to distribute.
  - Si maintenant , on a plusieurs (*n*) niveau d’énergie, le résultat est le produit de toutes les distributions

Number of energy levels

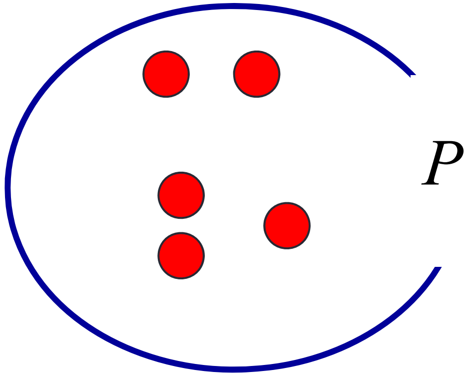
$$P = \prod_{i=1}^{n} \frac{g_i!}{N_i!(g_i - N_i)!}$$

Fermi –Dirac statistics

- Same approach than before



$$\frac{g_i!}{N_i!(g_i-N_i)!}$$



Number of energy levels

$$P=\prod_{i=1}^{\boxed{n}}\frac{g_i!}{N_i!(g_i-N_i)!}$$

Electrons density on energy level *E*

$$\boxed{f(E)=\frac{n(E)}{g(E)}=\frac{1}{1+\exp\left(\frac{E-E_F}{kT}\right)}}$$

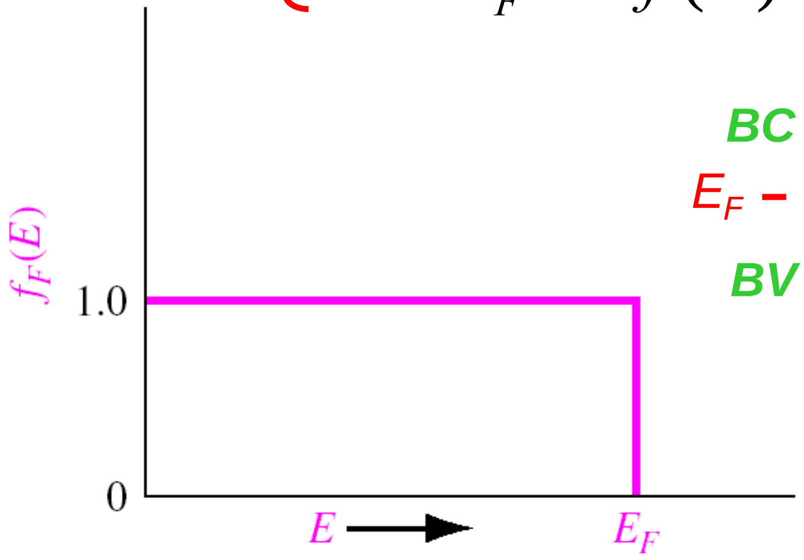
States density on energy level E

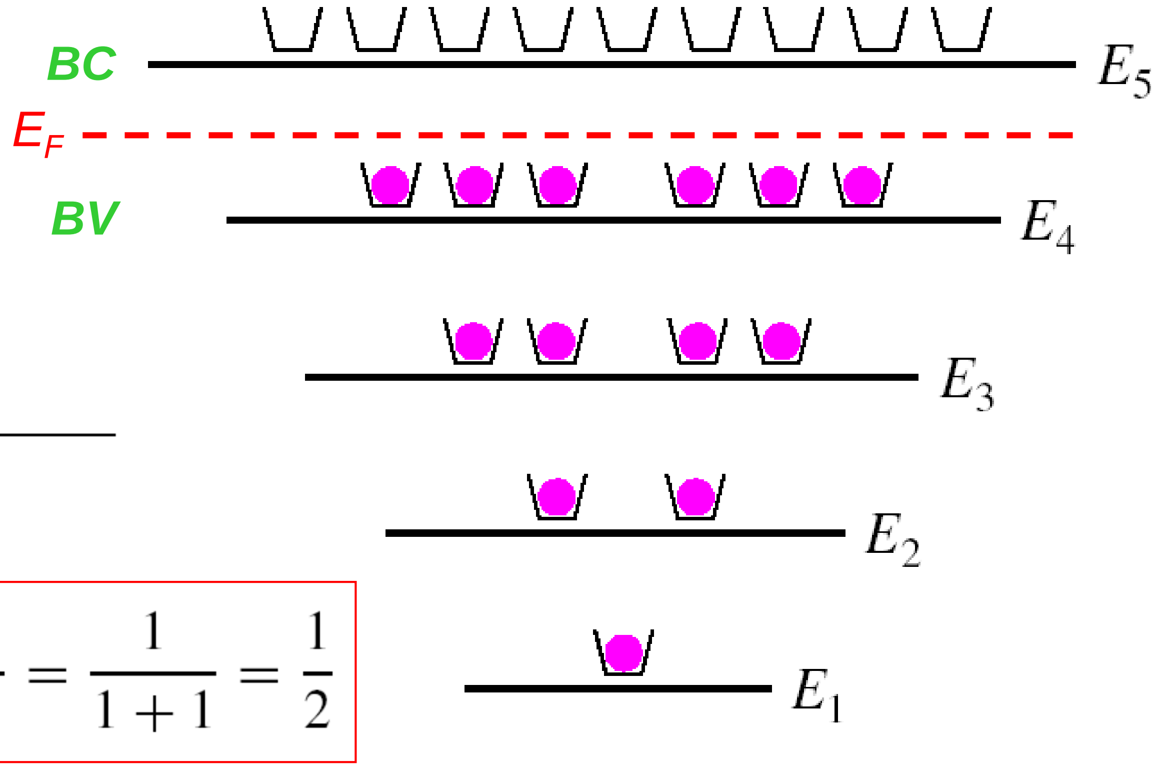
Fermi level

Fermi –Dirac statistics

at T= 0K: $\begin{cases} E < E_F \Rightarrow f(E) = 1 \\ E > E_F \Rightarrow f(E) = 0 \end{cases}$

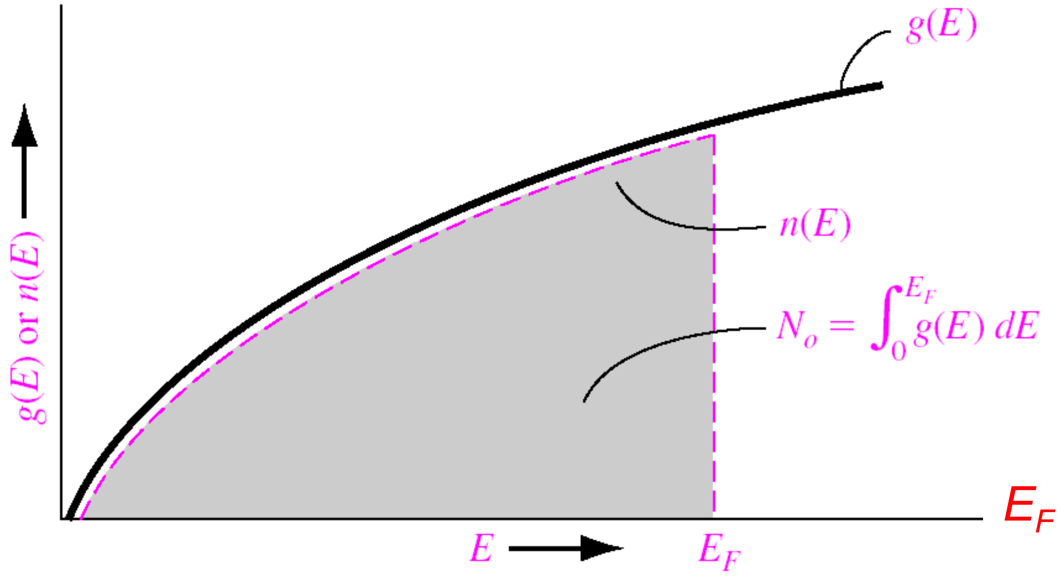
$$\boxed{f(E) = \frac{1}{1 + \exp\left(\dfrac{E - E_F}{kT}\right)}}$$





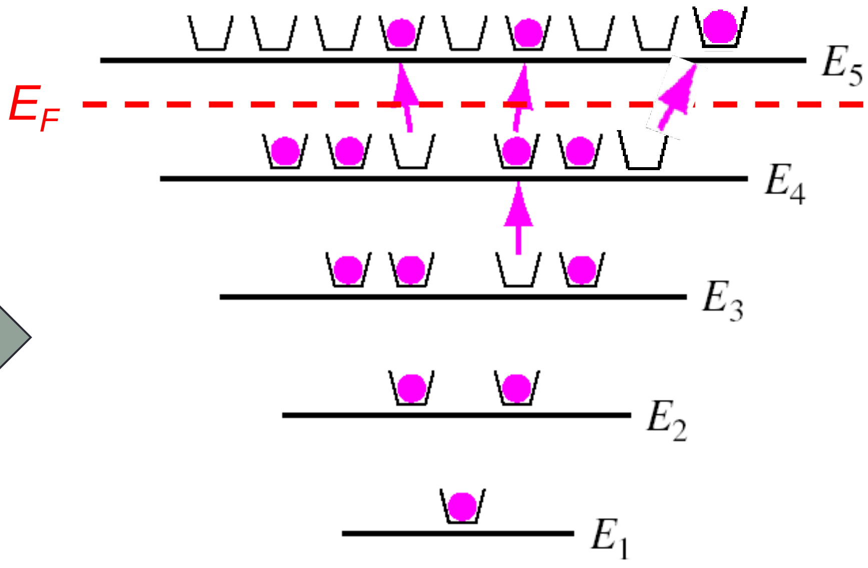
$$\boxed{f_F(E = E_F) = \frac{1}{1 + \exp(0)} = \frac{1}{1+1} = \frac{1}{2}}$$

Fermi –Dirac statistics

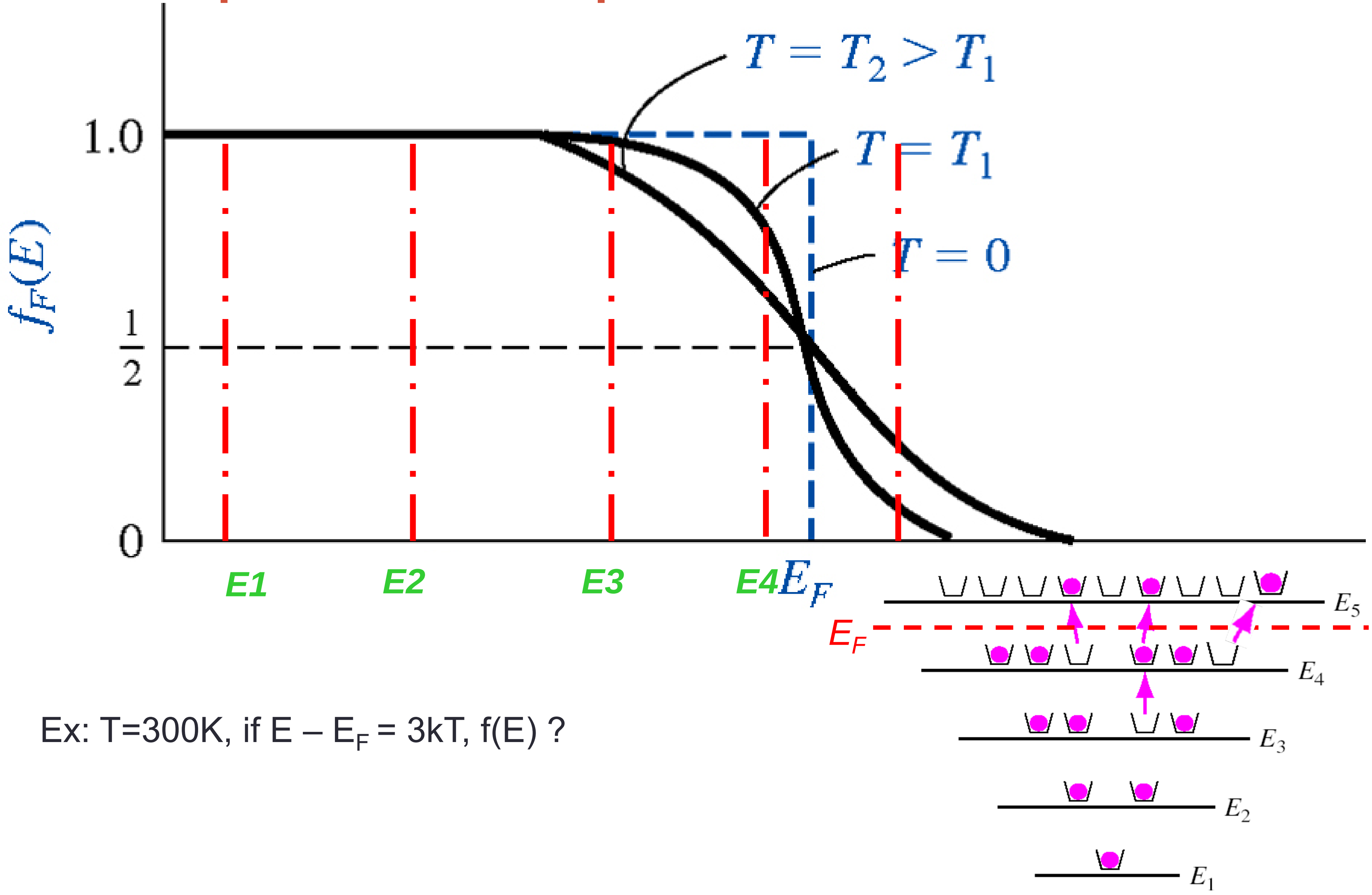


T = 0K

T> 0K



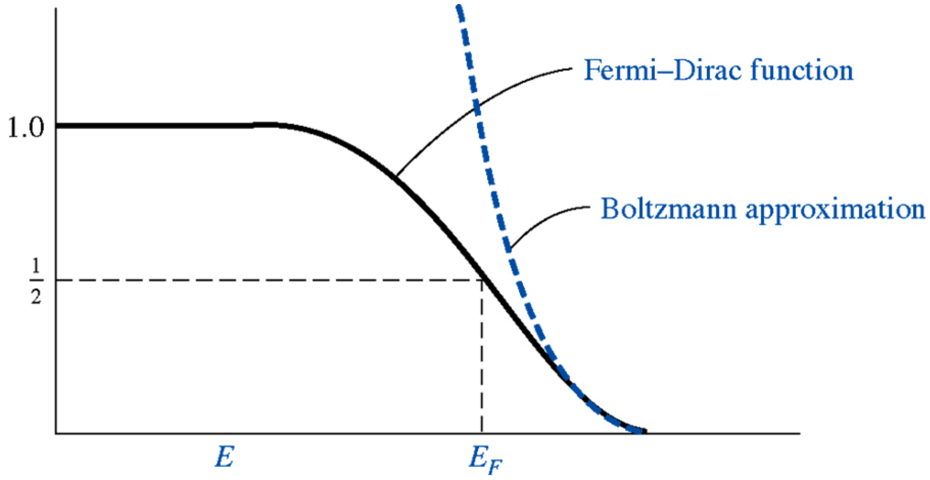
Temperature dependance



Ex: T=300K, if E – E_F = 3kT, f(E) ?

Approximation FD ⇔ MB ?

- The use of FD is not always easy in calculus
- In which conditions can we approximate FD by MB ?
  - Condition:

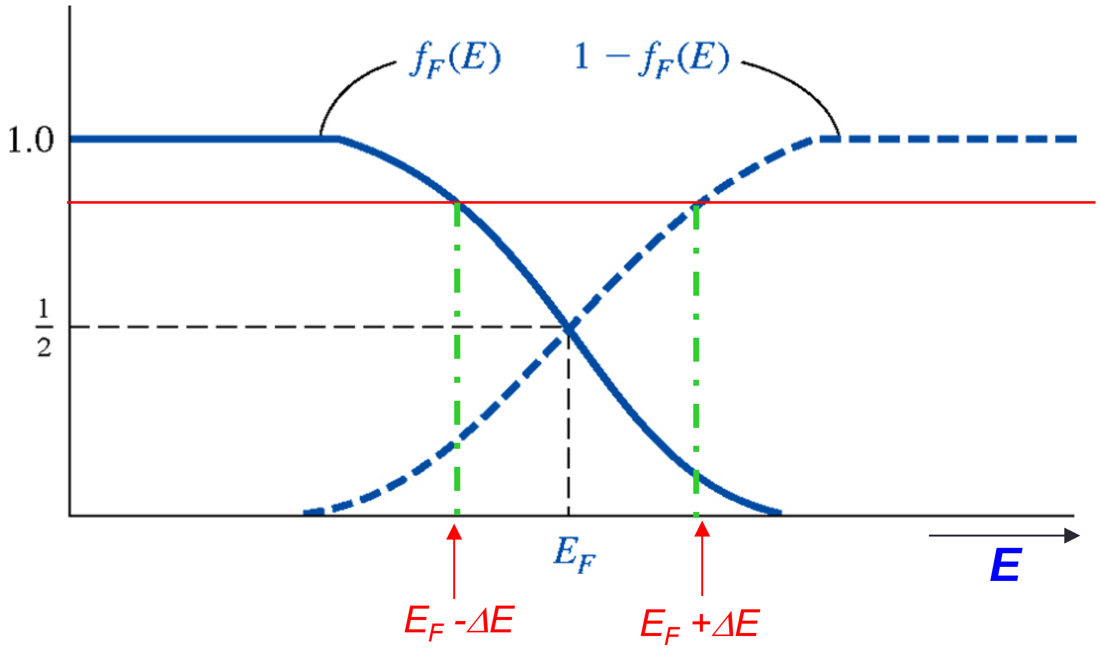


$$E - E_F \gg kT \quad \Rightarrow \quad f_F(E) \approx \exp\left[\frac{-(E - E_F)}{kT}\right]$$

Si E - E_F > 3 kT, 5% of error

- *Rule:* we can confound (5% error) Fermi – Dirac function and Maxwell – Boltzmann function when | E - E_F |> 3kT. At room temperature (T=300K), kT=25 meV ⇔ | E - E_F |> 75 meV.

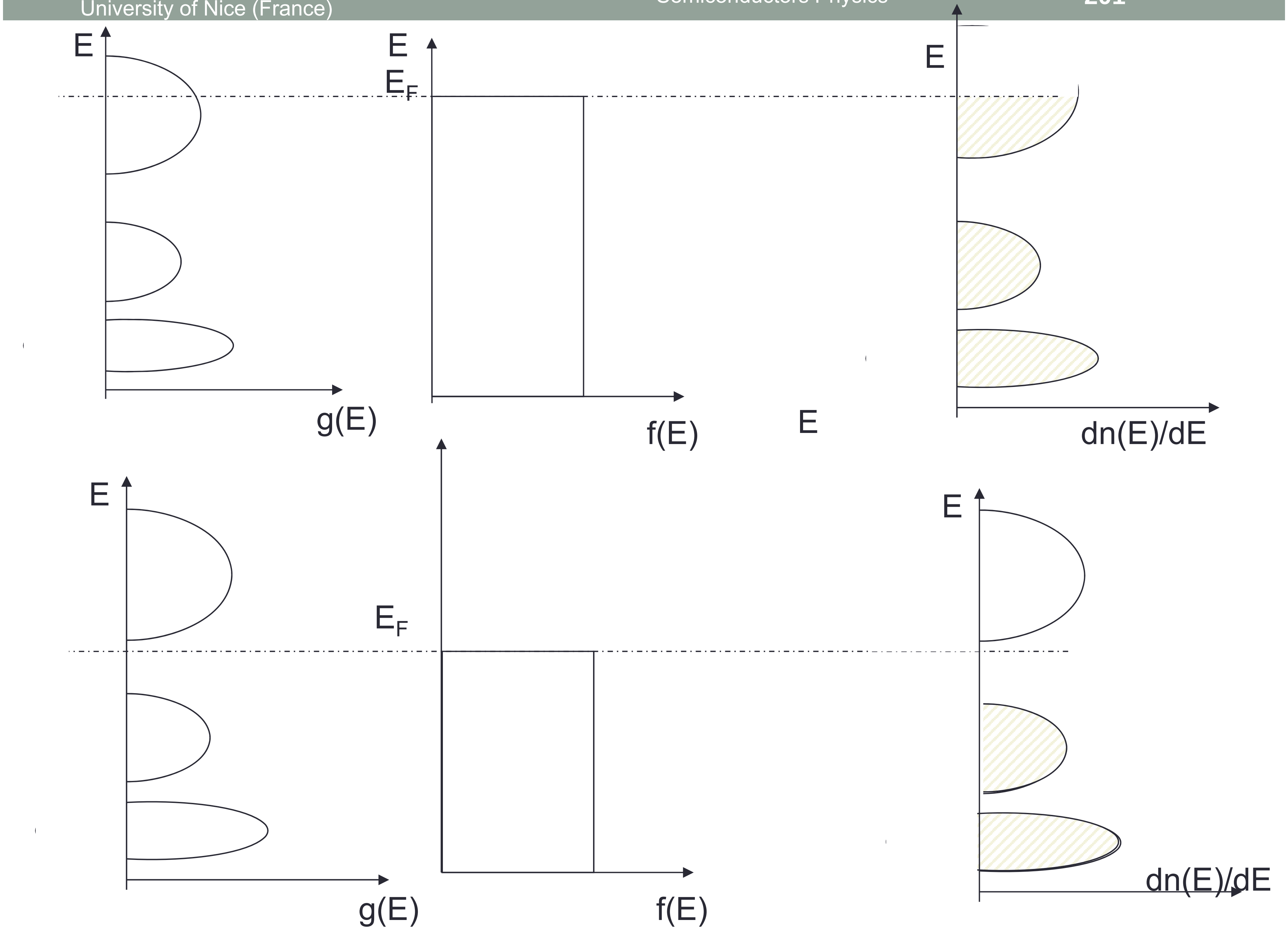
Approximation FD ⇔ MB ?



For $E < E_F$, it's easy to show that the unoccupation probility 1-f(E) is the same at $E_F - \Delta E$ than the occupation probability f(E) at $E_F + \Delta E$.

$$1 - f(E_F - \Delta E) = f(E_F + \Delta E)$$

The point f(E) = 0,5 is the center of symmetry for the curve.


E
g(E)
E
E_F
f(E)
E
E
dn(E)/dE
E
g(E)
E_F
f(E)
E
dn(E)/dE

CHAPTER 10

The semiconductor in equilibrium

The semiconductor in equilibrium

- equilibrium?
  - No external forces:
    - No applied voltage
    - No magnetic field
    - No gradient of temperature

Charge carrier density in semiconductor.

- *Question*: how many electrons in CB and holes in VB in a semiconductor at a given temperature ?
- *answer :* (see chap 9!)
  - At an energy E:

$$n(E) = g_c(E) f(E)$$

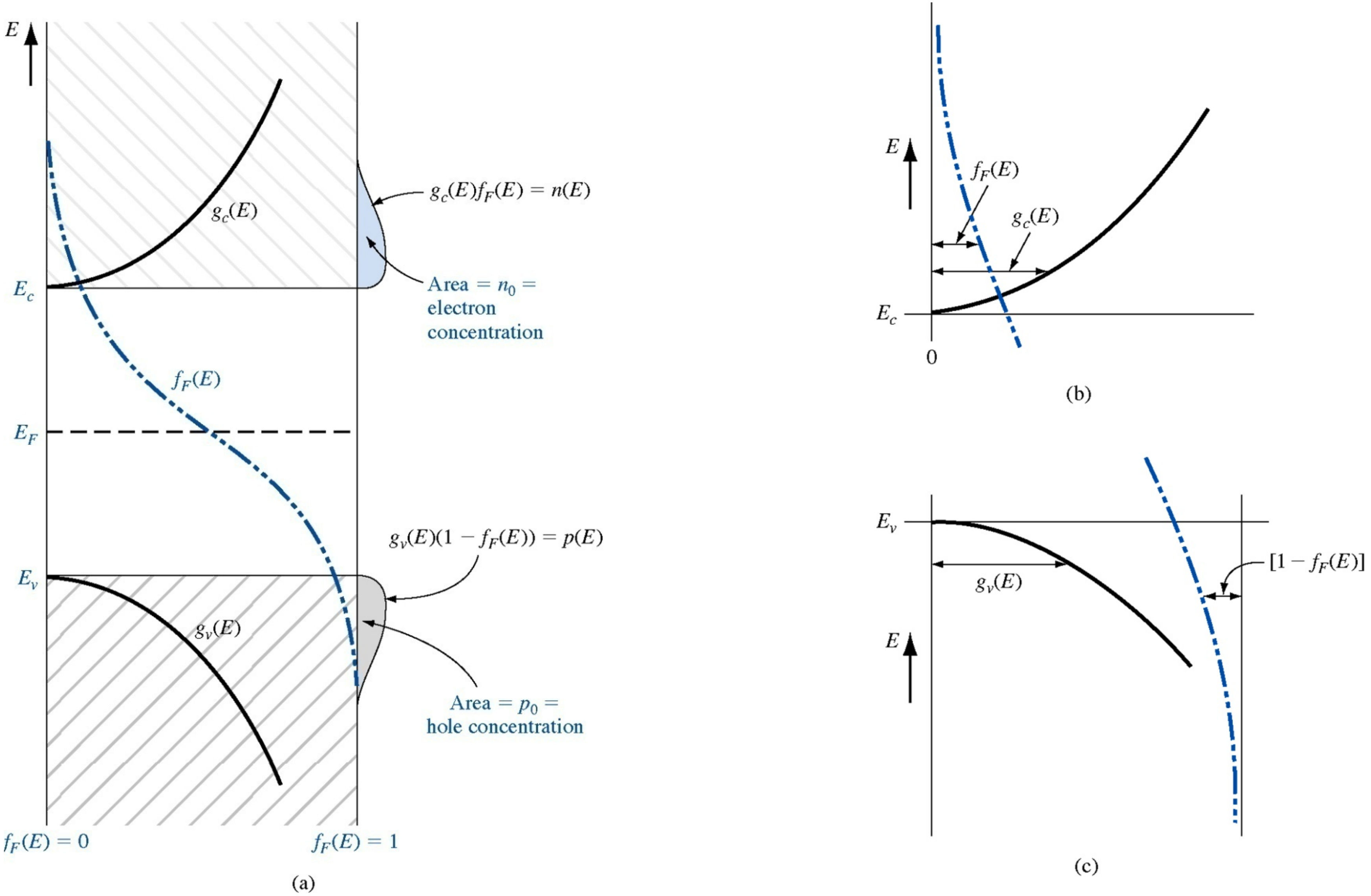
$$p(E) = g_v(E)(1 - f(E))$$

  - In a band with a given width

$$n_0 = \int_{Ec\min}^{Ec\max} g_c(E) f(E) dE$$

$$p_0 = \int_{Ev\min}^{Ev\max} g_v(E)(1 - f(E)) dE$$

Charge carrier density in semiconductor.



(a)

(b)

(c)

n_0 and p_0 equations

- <u>hypothesis:</u> E_F is 3kT (or more) below CB and is 3KT above BV ⇔ we can use MB function.
  - *n_0 relations:*

$$n_0 = \int_{Ec\min}^{Ec\max} g_c(E)f(E)dE = \int_{Ec\min}^{+\infty} \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E-E_C}\times e^{-(\frac{E\ -E_F}{kT})}dE$$

$$n_0 = \boxed{N_C \exp\left[\frac{-(E_c-E_F)}{kT}\right] \quad \text{avec} \quad N_C = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}}$$

n_0 and p_0 equations

$$n_0 = N_C \exp\left[\frac{-(E_c - E_F)}{kT}\right] \quad \text{with} \quad N_C = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$$

$$p_0 = N_V \exp\left[\frac{-(E_F - E_v)}{kT}\right] \quad \text{with} \quad N_V = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}$$

N_c and N_v are the effective density of states function (~ density of place) in the conduction band and valence band respectively. The magnitde is around Nc ~ Nv ~ 2.5 x 10^{19} cm^{-3}.

It is as if all the energy states in the CB were effectively squeezed into a single energy level, E_C or E_v

Law of mass action

- *Pratical rule*: if we take the product of electrons density in the CB and holes density in the VB, we obtain:

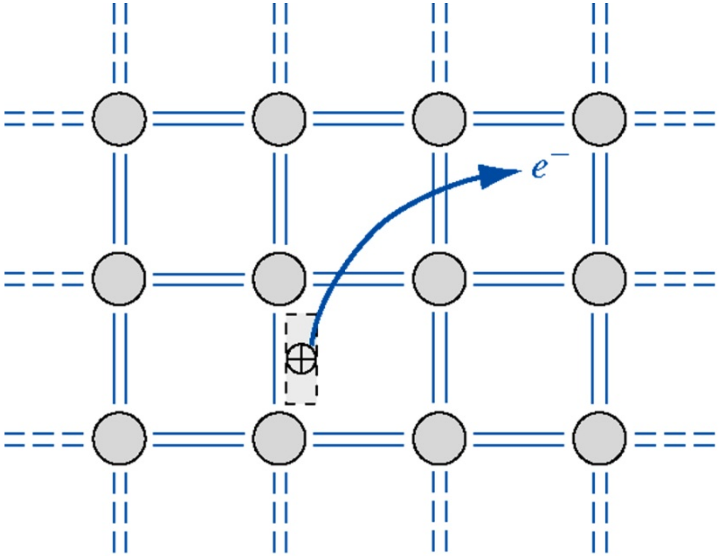
$$\boxed{n \times p = N_c N_v \exp(-\frac{E_c - E_v}{kT}) = N_c N_v \exp(-\frac{E_g}{kT}) = n_i^2}$$

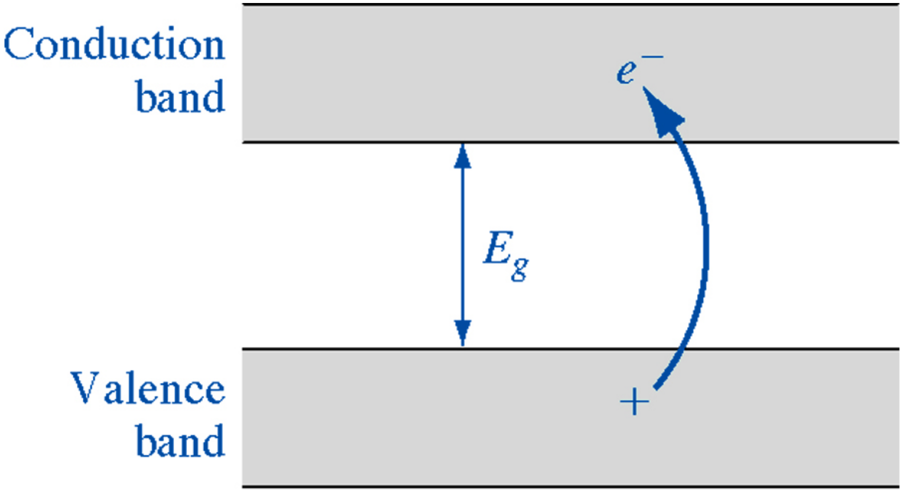
- *Important remark*: the expressions we have just established for n and p have been assuming that EF is separated from CB and VB by at least 3kT. This calculation does not assume that n = p ⇔Rule $n \times p = n_i^2$ will remain true even when the SC will be doped, provided the condition on EF is valid. Otherwise (exception) we say that the SC is degenerate.

Fermi level in an intrinsic semiconductor

- Intrinsic semiconductor : free impureties semiconductor, *ie* only allowed energy level are the CB and the VB.
- n electrons in the CB . These electrons come from VB. It leads to p holes in the VB and of course:

$$\boxed{\Rightarrow n = p = n_i \qquad \forall T}$$





Fermi level in an intrinsic semiconductor

- Postulat: *n* = *p*

$$n_0 = N_C \exp\left[\frac{-(E_c - E_{F_i})}{kT}\right] = p_0 = N_V \exp\left[\frac{-(E_{F_i} - E_v)}{kT}\right]$$

⬇

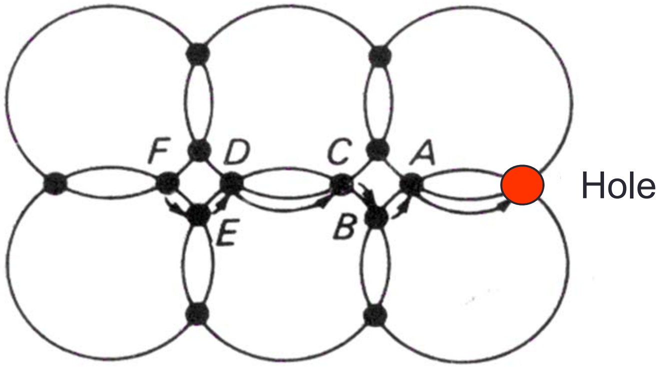
$$\exp\left[\frac{2E_{F_i}}{kT}\right] = \frac{N_C}{N_V}\exp\left[\frac{(E_c + E_v)}{kT}\right]$$

⬇

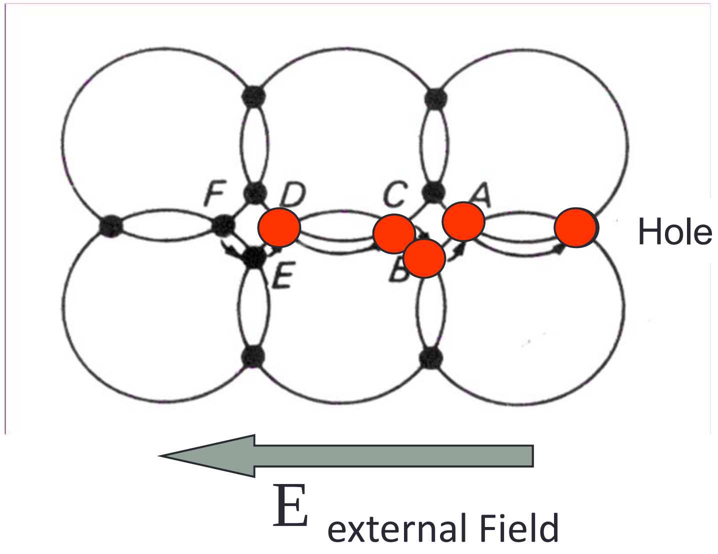
$$\boxed{E_{F_i} = \frac{E_c + E_v}{2} + \frac{1}{2}kT\ln\frac{N_V}{N_C} = \frac{E_c + E_v}{2} + \underbrace{\frac{3}{4}kT\ln\frac{m_v^*}{m_c^*}}_{\sim 10\ \text{meV}} \cong \boxed{\frac{E_c + E_v}{2} = E_{F_i}}}$$

Bipolar conduction

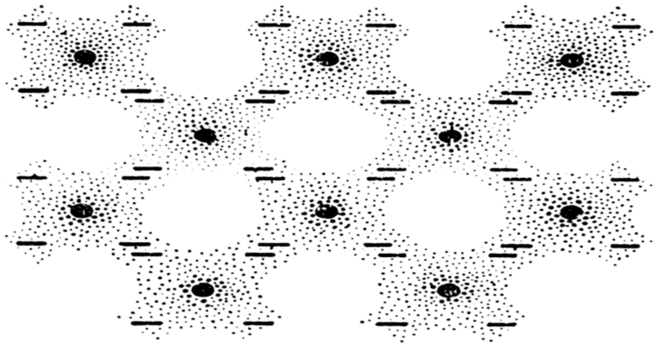
- The presence of electrons and holes causes bipolar conduction in the SC



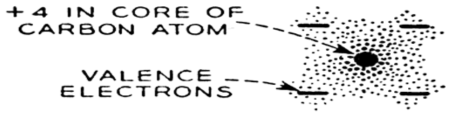
- By adding a small amounts of specific dopants, we can alter the conduction process and we can favor conduction by electrons or holes



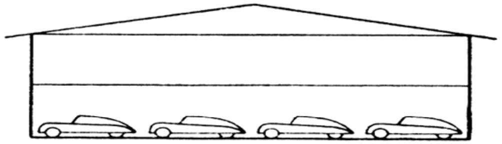
Electrons in a diamond structure (ex: Si)



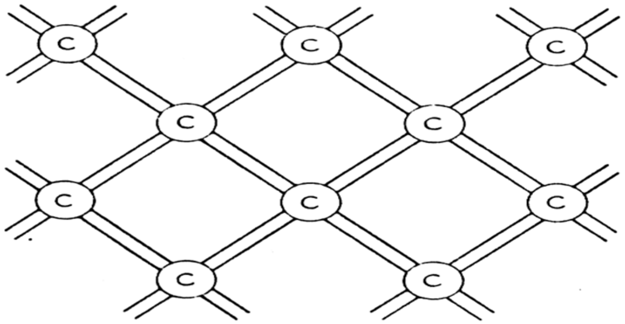
(a) ELECTRON PAIR BONDS



(b)

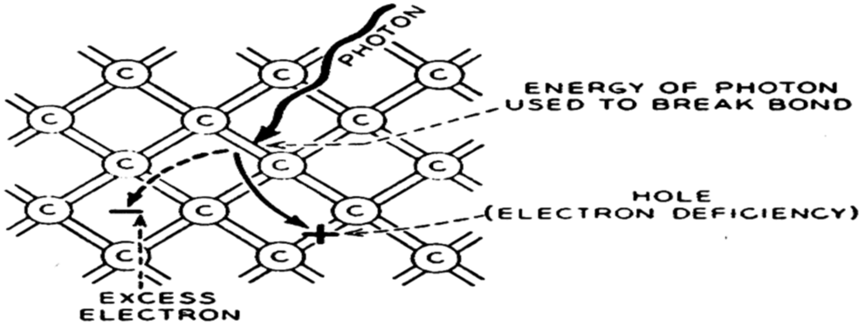


NO TRAFFIC POSSIBLE

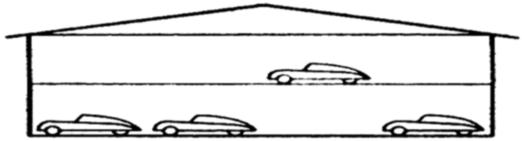


(C) PLANE DIAGRAM OF DIAMOND LATTICE WITH BONDS REPRESENTED BY LINES

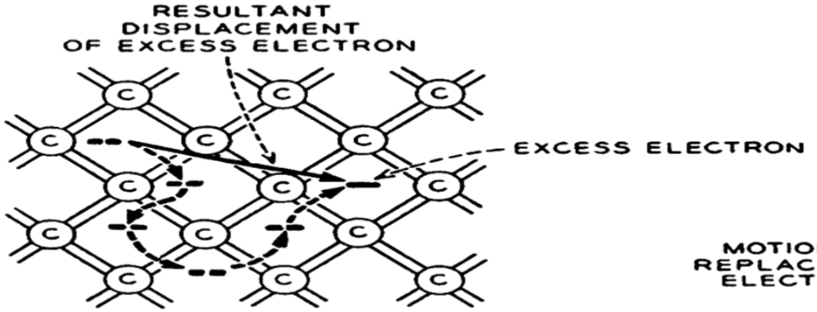
Electrons in a diamond structure (ex: Si)



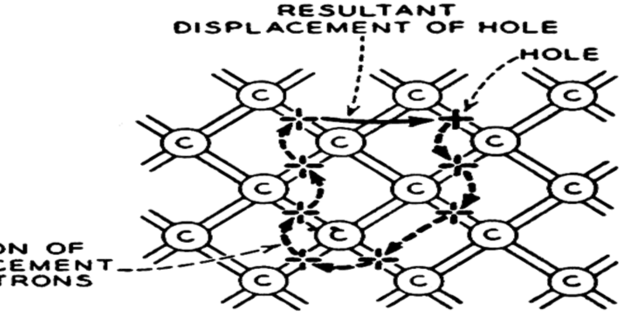
(a) PRODUCTION OF A HOLE-ELECTRON PAIR BY A PHOTON



(b) TRAFFIC POSSIBLE



(C) RANDOM MOTION OF AN EXCESS ELECTRON



(d) RANDOM MOTION OF A HOLE

Some semiconductors

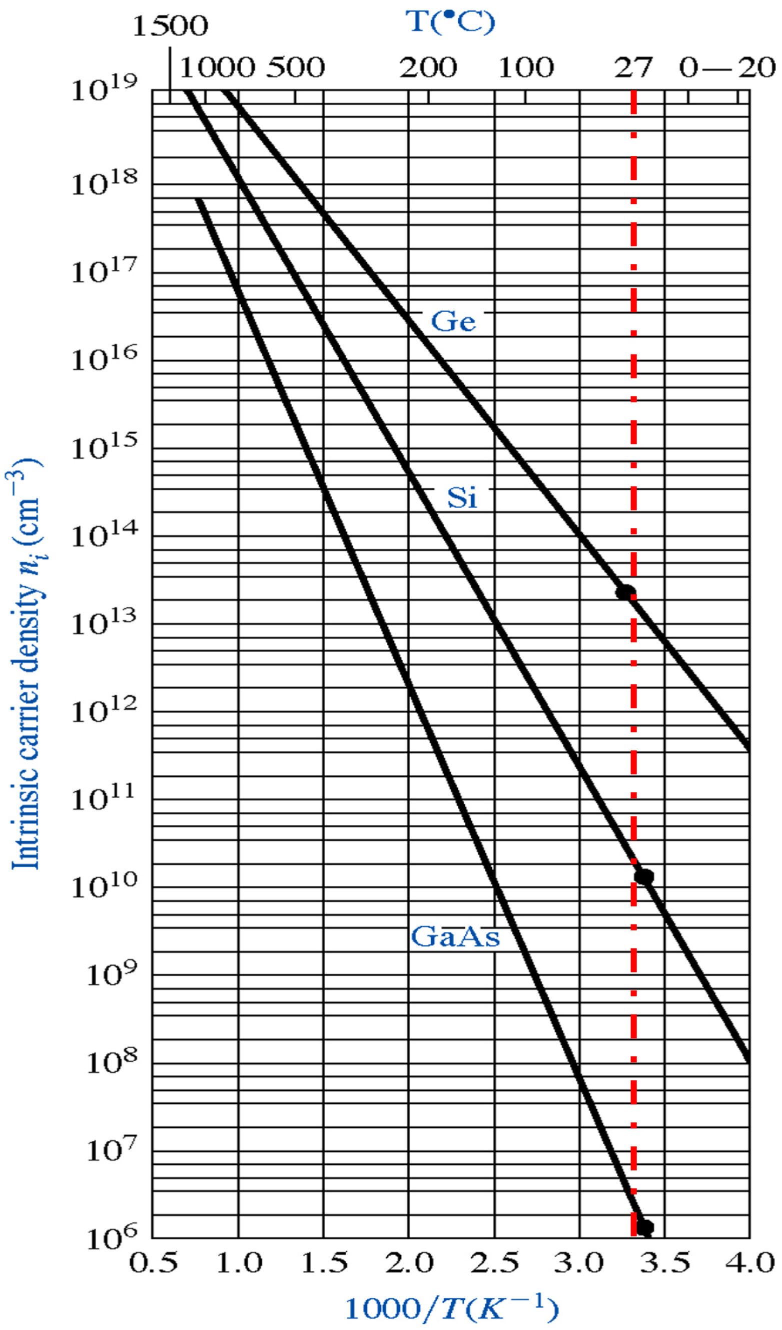
- Data (300K):

	${m_c^*}/{m_0}$	${m_v^*}/{m_0}$	N_C (10^{19} cm^{-3})	N_V (10^{19} cm^{-3})	Eg (eV)	n_i (cm^{-3})
Si	1,06	0,59	2,7	1,1	1,12	$1{,}5\mathrm{x}10^{10}$
Ge	0,55	0,36	1	0,5	0,66	$2{,}4\mathrm{x}10^{13}$
GaAs	0,067	0,64	0,04	1,3	1,43	$2\mathrm{x}10^{6}$
GaN	0,2	1,4	0,223	4,6	3,39	
4H-SiC			1,69	2,49	2,86	
InP	0,073	0,87	0,05	2	1,27	

n_i as a function of temperature

$$n_i = \sqrt{N_c N_v}\exp\left(-\frac{E_g}{2kT}\right)$$

- In an intrinsic SC:
  - n_i is not a constant
  - n_i increases as:
    - E_g decreases
    - Temp increases



Doping of semiconductors

- Exponential variation of the intrinsic carrier density
- If $n_i > 10^{15} cm^{-3}$, the semiconductor is not suitable for electronic devices
- We can decrease n_i by using large band gap material (SiC, GaN, Diamond)

- Remark: $n \times p$ product is independant of Fermi level (except Boltzmann approximation is valid) ⇔ valid even the SC is doped

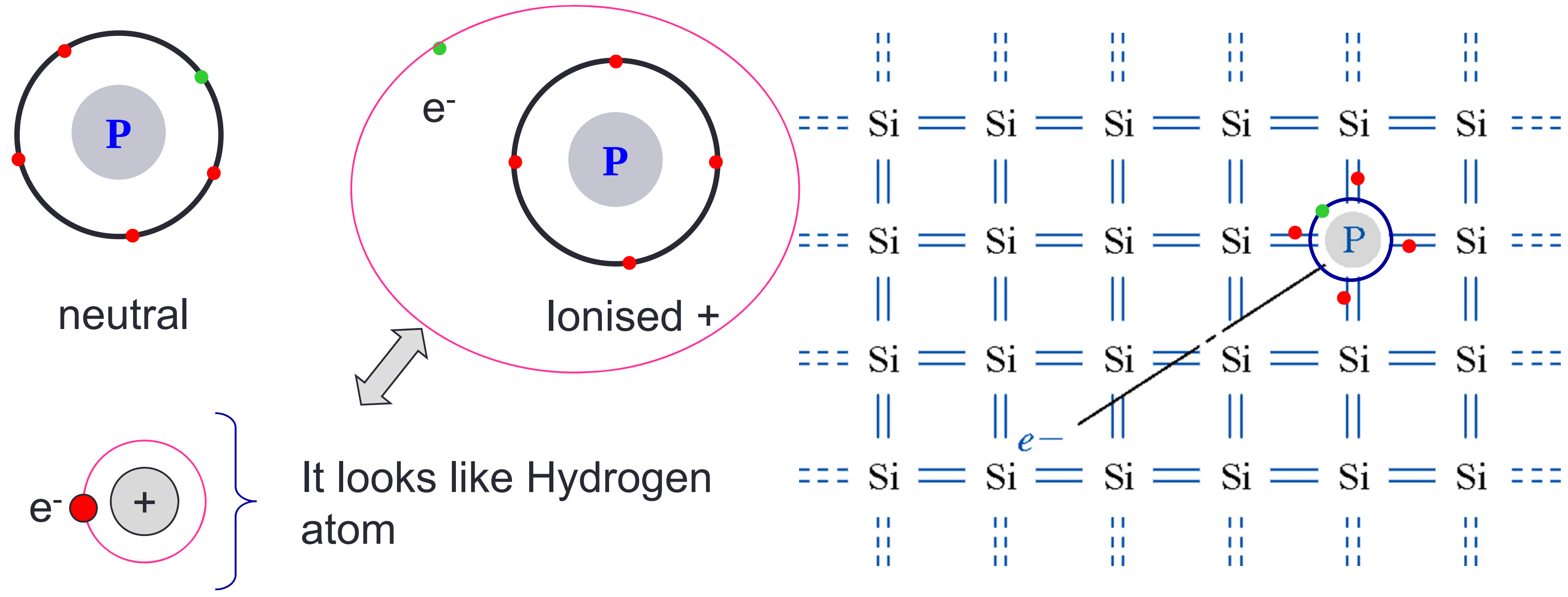
Semiconductor doping

- Allow to change and control electrical properties of semiconductor
- Doping impurities will change the relation $n = p$:
  - Donor like impurety ⇔ n > p ⇔ n type
  - Acceptor like impurety ⇔ p > n ⇔ p type

Depending of the nature of the chemical species (position in the periodic table), the behavior of these impureties will favor n type conduction or p type conduction.

Semiconductor doping

- Case of Silicon (col IV)
  - If we introduce doping impureties from column V:
    - For example N, As or P ⇔ 5 valence electrons *ie* one extra electron compared to the Silicon.



It looks like Hydrogen atom

Semiconductor doping

- Column V atom : analogy with the hydrogen atom
  - The extra electron does not belong to VB !
  - The extra electron does not belong to CB !
  - Where is its energetic position? Between the both of them !!

- Midified hydrogen model »:
  - Electron is not moving in a free space
  - Electron has an effective mass (different of the free mass)

⇓

We will now calculate this energetic position

Ionization energy of dopants.

- *Force*

$$F = \frac{1}{4\pi\varepsilon_0\varepsilon_{vacuum}}\frac{q^2}{r^2}$$

- *Potential*

$$V = -\frac{1}{4\pi\varepsilon_0\varepsilon_{vacuum}}\frac{q}{r}^2$$

- *Energy*

$$E_n = -\frac{mq^4}{2n^2(4\pi\varepsilon_0\varepsilon_{vacuum}\hbar)^2}$$

- *Rydberg*

$$R = \frac{mq^4}{2(4\pi\varepsilon_0\varepsilon_{vacuum}\hbar)^2} = 13{,}6eV$$

We have to replace:

- ε_{vaccum} by ε_{sc}
- *m* by *m**.

$$R_y^* = R_y \frac{1}{\varepsilon_{sc}^2}\frac{m*}{m_0}$$

Donnor level in the forbidden energy band (gap).

- *Application to Silicon* (ε_{Si}~12)
  - In our case, E is energy we have to give to electron to elevate it (the extra electron) into the conduction band.
  - $E = E_C - E_D = R_y^*/n^2 = R_y^*$

$$\boxed{R_y^* = 13{,}6 \frac{1}{(12)^2} \frac{0{,}5 \times m_0}{m_0} \approx 40 meV}$$

  - Experimental measurements :

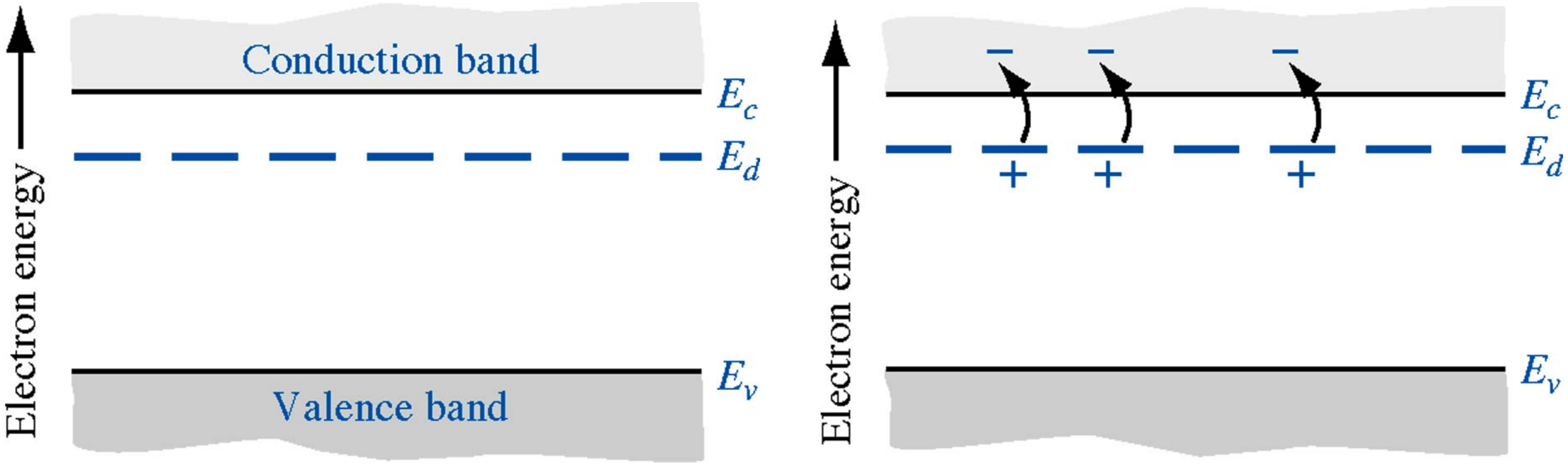
P	=>	44 meV
As	=>	49 meV
Sb	=>	39 meV
Bi	=>	67 meV

Donor level in the forbidden energy band (gap).

- *Summary :*
  - When the extra electron is bonded to P atom ⇔ energy level E_D and its orbit are localized around the donor atom.
  - When the electron moves to conduction band ⇔ its quantum state changes (quantum state describes by Bloch wave)) ⇔ it's moving in the crystal ⇔ it contributes to the conduction, it is a free electron

- *compounds SC*
  - *GaAs or InP (III-V)*
    - VI substitutes to As => Se, Te
    - IV substitutes to Ga => Si, C, Sn
    - $m^*=0,05\ m_0$ ⇔ $E_C - E_D = 5$ meV !!

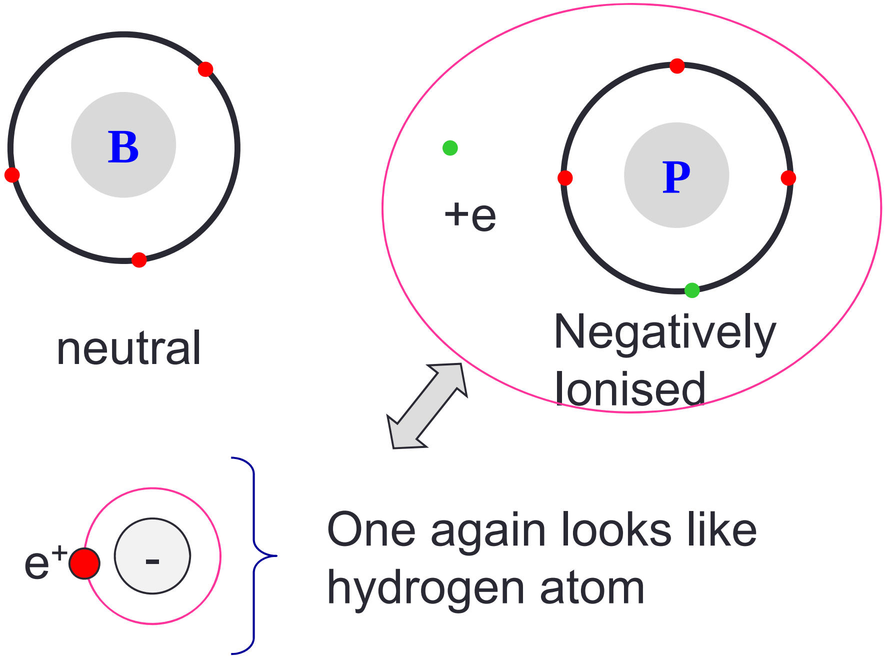
Donor level in the forbidden energy band (gap).



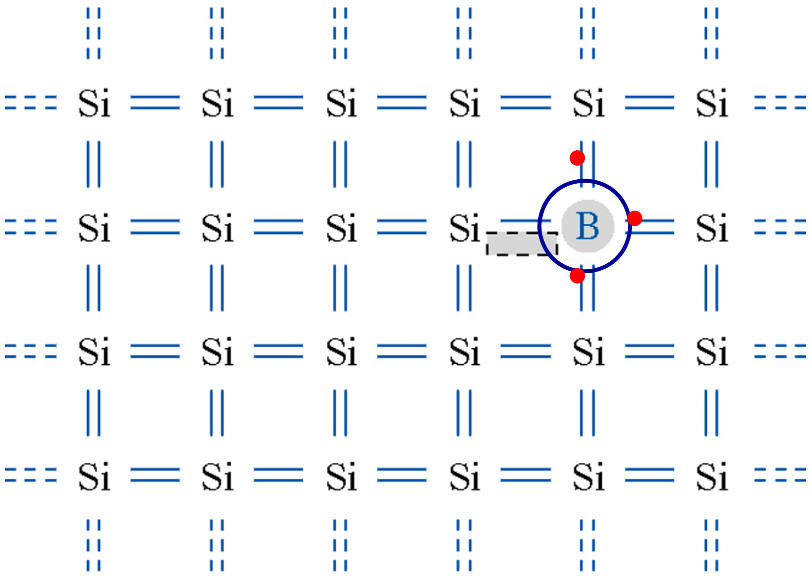
- we can create / elevate electrons in CB without any holes in VB ⇔ *n >> p.*
- VB is full ⇔ no conduction allowed in this band.
- only charge carriers in CB (electrons) conduct ⇔ unipolar conduction

Acceptor level in the forbidden energy band (gap)..

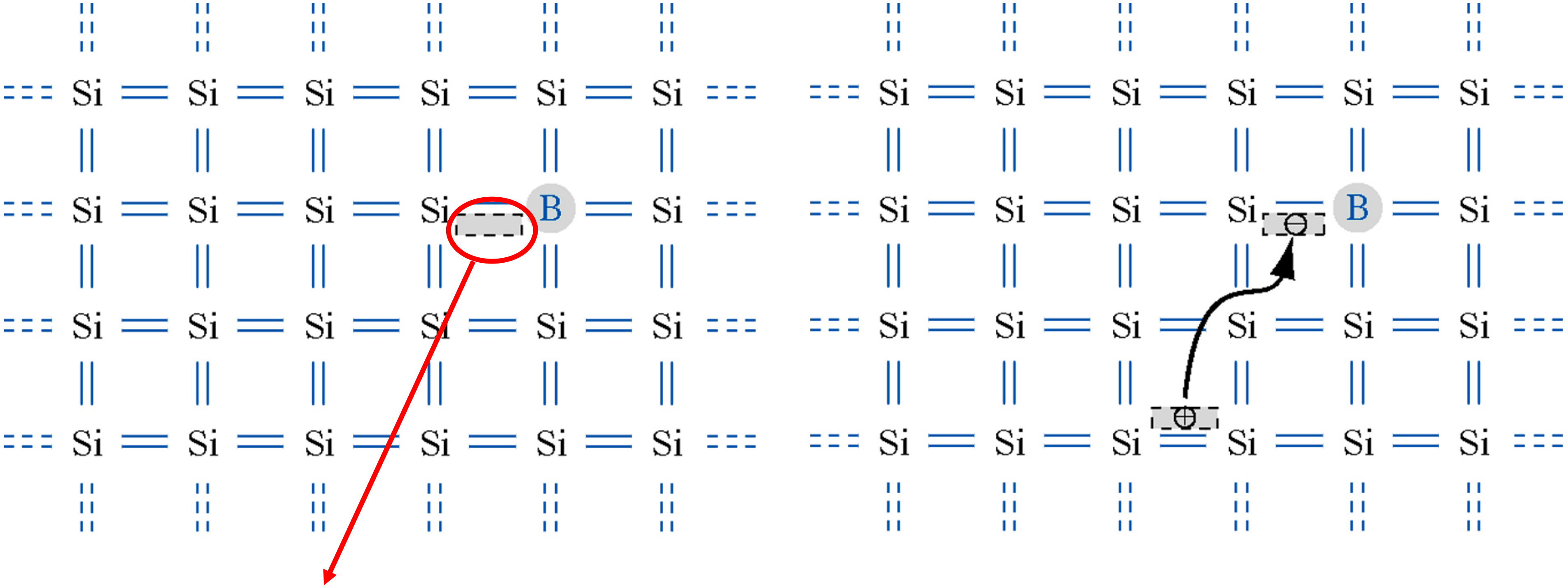
- Case of Silicon (col IV)
  - If we introduce doping impureties from column III:
    - For ex B, Al ou Ga ⇔ 3 valence electrons *ie* one fewer compared to Si.



One again looks like hydrogen atom



Acceptor level in the forbidden energy band (gap)..



Free quantum state: we can show that this energy level is very close to the valence band. Same calculation than « donor » level.

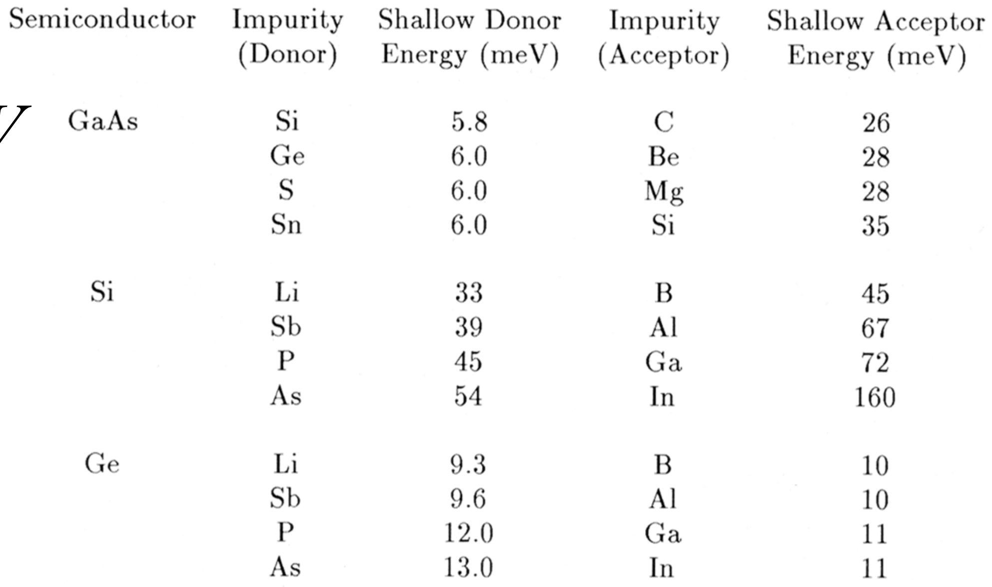
How to calculate the energy level E_d or E_a

- The problem "looks like" the model of the hydrogen atom :

$$E_n = \frac{\underline{m}_0 e^4}{2(4\pi\underline{\varepsilon_0})^2\hbar^2} = \frac{13.6}{n^2}eV$$

- Introduction of modified Rydberg:

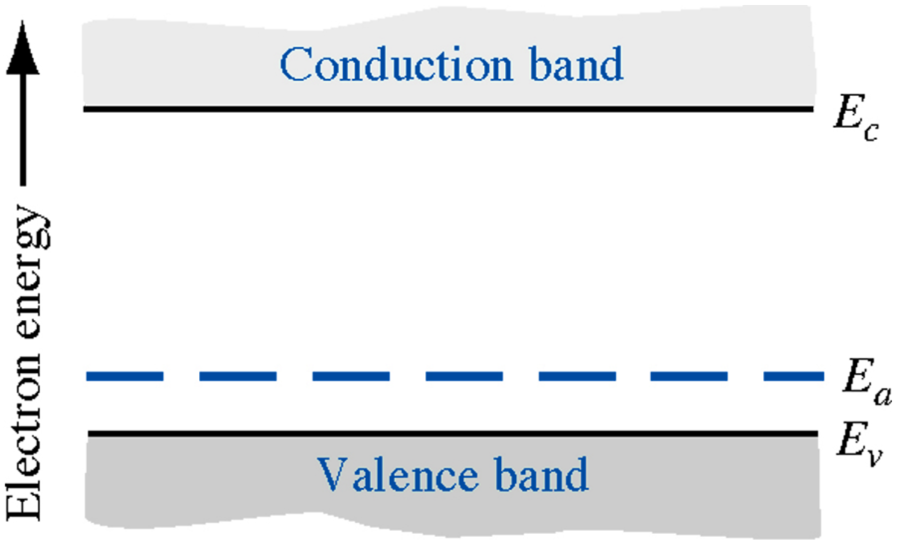
$$E_d = E_C - 13.6\left(\frac{m^*}{m_0}\right)\left(\frac{\varepsilon_0}{\varepsilon}\right)^2$$

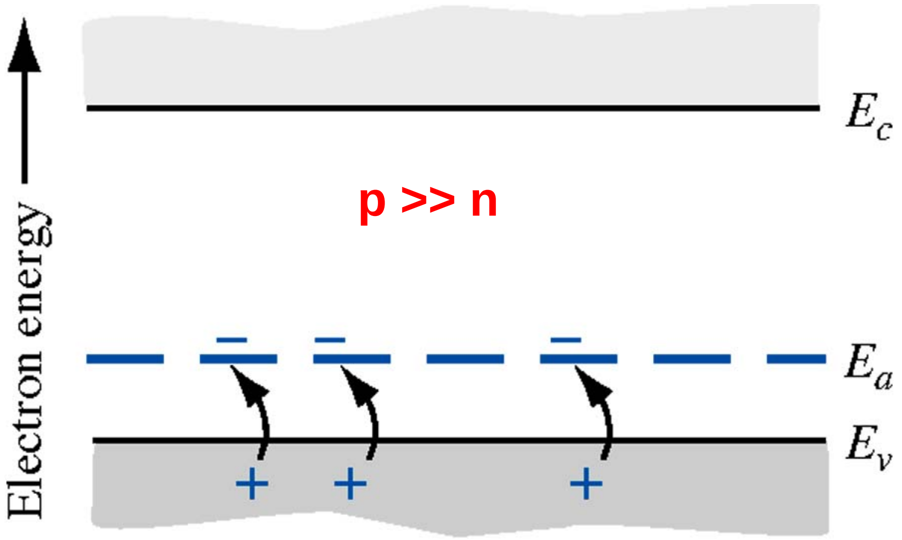


Semiconductor	Impurity (Donor)	Shallow Donor Energy (meV)	Impurity (Acceptor)	Shallow Acceptor Energy (meV)
GaAs	Si	5.8	C	26
	Ge	6.0	Be	28
	S	6.0	Mg	28
	Sn	6.0	Si	35
Si	Li	33	B	45
	Sb	39	Al	67
	P	45	Ga	72
	As	54	In	160
Ge	Li	9.3	B	10
	Sb	9.6	Al	10
	P	12.0	Ga	11
	As	13.0	In	11

Few examples

Acceptor level in the forbidden energy band (gap)..





$$\boxed{E_a - E_V = \frac{13{,}6}{\varepsilon_{sc}^2}\,\frac{m_v^*}{m_0}}$$

- We get :
  - B => 45 meV
  - Al => 57 meV
  - Ga => 65 meV
  - In => 160 meV

Statistics for donor and acceptor levels

- Donor states:
  - The writing has to be lightly modified:

$$f_D(E) = \frac{1}{1 + \frac{1}{2}\exp(\frac{E - E_F}{kT})}$$

  - Factor ½ ?
    - P : $3s^2 3p^3$ ⇔ 2 electrons *s* and 2 électrons *p* participate in the bindind=> the extra electron (*p* state) are on the E_d level. This electron has a particular spin value (up ou down).
    - Once that an electron leaves this level, the box (the level) is empty and can trap a up or down spin ⇔ the capture mechanism is increased compared to the emission one

$$f_D(E) > f(E)$$

Statistics for donor and acceptor levels

- Donor states:
  - Electrons density trapped on E_D ?

$$n_D = N_D \times f_D(E_D) = \frac{N_D}{1+\frac{1}{2}\exp(\frac{E_D - E_F}{kT})}$$

  - Or :

$$n_d = N_d - N_d^+$$

Statistics for donor and acceptor levels

- Acceptor level:
  - One can only capture the electron that has the right "spin" but we can release any ⇔ $f_A(E) < f(E)$

$$f_A(E) = \frac{1}{1 + 2\exp(\frac{E - E_F}{kT})}$$

$$f(E) = \frac{1}{1 + g\exp(\frac{E - E_F}{kT})}$$

g : degeneracy factor

1 : intrinsic
2 ou 4: acceptor
½: donor

Statistics for donor and acceptor levels

- Acceptor level:
  - Electron density on E_A

$$n_A = N_A \times f_A(E_A) = \frac{N_A}{1 + 4\exp(\frac{E_A - E_F}{kT})}$$

  - or:

$$p_A = N_A - n_A = N_A - N_A^- = \frac{N_A}{1 + \frac{1}{4}\exp(\frac{E_F - E_A}{kT})}$$

Total ionization and carriers freeze out

- Neutrality relation:
  - Positive charges = negative charges

$$e\left(p+N_D^+\right)=e\left(n+N_A^-\right)$$

  - Simplification : $N_A = 0$ (n type)

$$n-p=N_D^+$$

$$N_C \exp\left[\frac{-(E_c-E_F)}{kT}\right] - N_V \exp\left[\frac{-(E_F-E_v)}{kT}\right] = \frac{N_D}{1+2\exp(-\frac{E_D-E_F}{kT})}$$

Fermi level $E_F(T)$

- We “split” of the problem in the temperature range :
  - ULT (ultra low temperature) : we neglect the holes ; OK but until which temperature this assumption is correct?

$$n_i << N_D \qquad \Leftrightarrow \qquad kT << \frac{E_g}{2\ln[(NcNv)^{1/2}/N_D]}$$

kT must be around Eg/10

$$\Rightarrow \qquad N_C \exp\left[\frac{-(E_c - E_F)}{kT}\right] - \frac{N_D}{1 + 2\exp(\frac{E_D - E_F}{kT})} = 0$$

Fermi level $E_F(T)$

⇨ $$E_F = E_D + kT\ln\left\{\frac{1}{4}\left[\enclose{circle}{-1} + \left(\enclose{circle}{1} + 8\frac{Nd}{Nc}e^{(Ec-Ed)/kT}\right)^{1/2}\right]\right\}$$

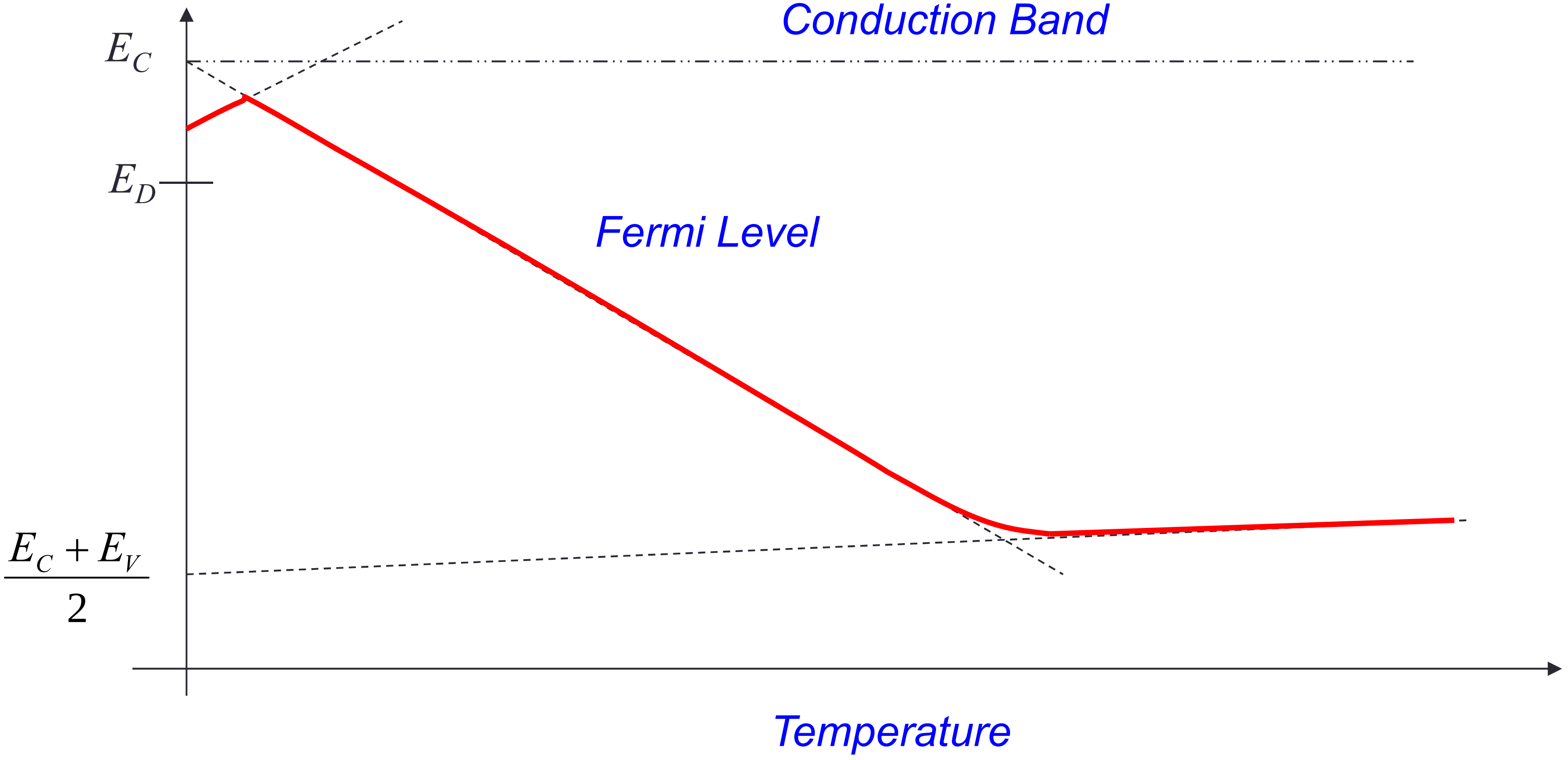
- $kT \ll E_c - E_d$

$$E_F = \frac{E_c + E_d}{2} + \frac{1}{2}kT\ln\frac{N_d}{2N_C} \quad , \; E_F(\mathrm{T}=0) = \frac{E_c + E_d}{2} \quad E_F^{\max} \Rightarrow N_C = N_D/2$$

- $E_c - E_d < kT < Eg$

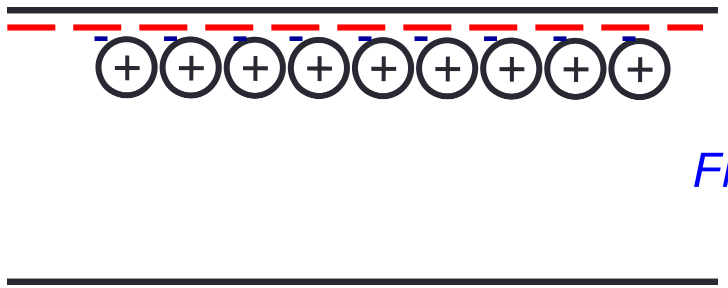
⇨ (Taylor’s series of the square root) $$E_F = E_c - kT\ln\frac{N_C}{N_D}$$

E_F function of the Température



And the carrier density ?

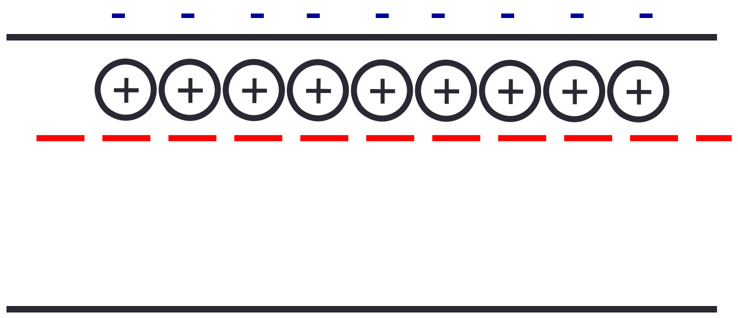
- LT



Freeze out *(« gel des porteurs »)*

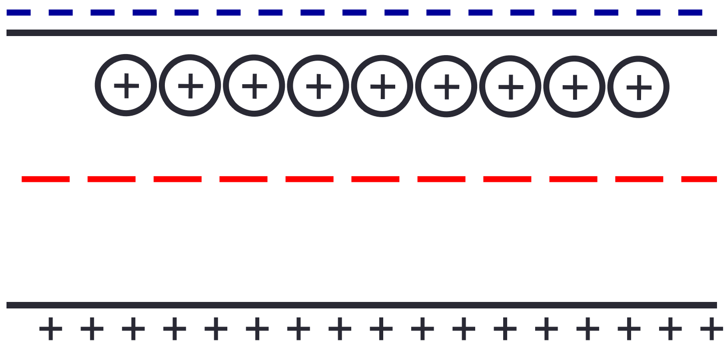
- T « middle range »

  Exhaustion/saturation of donors

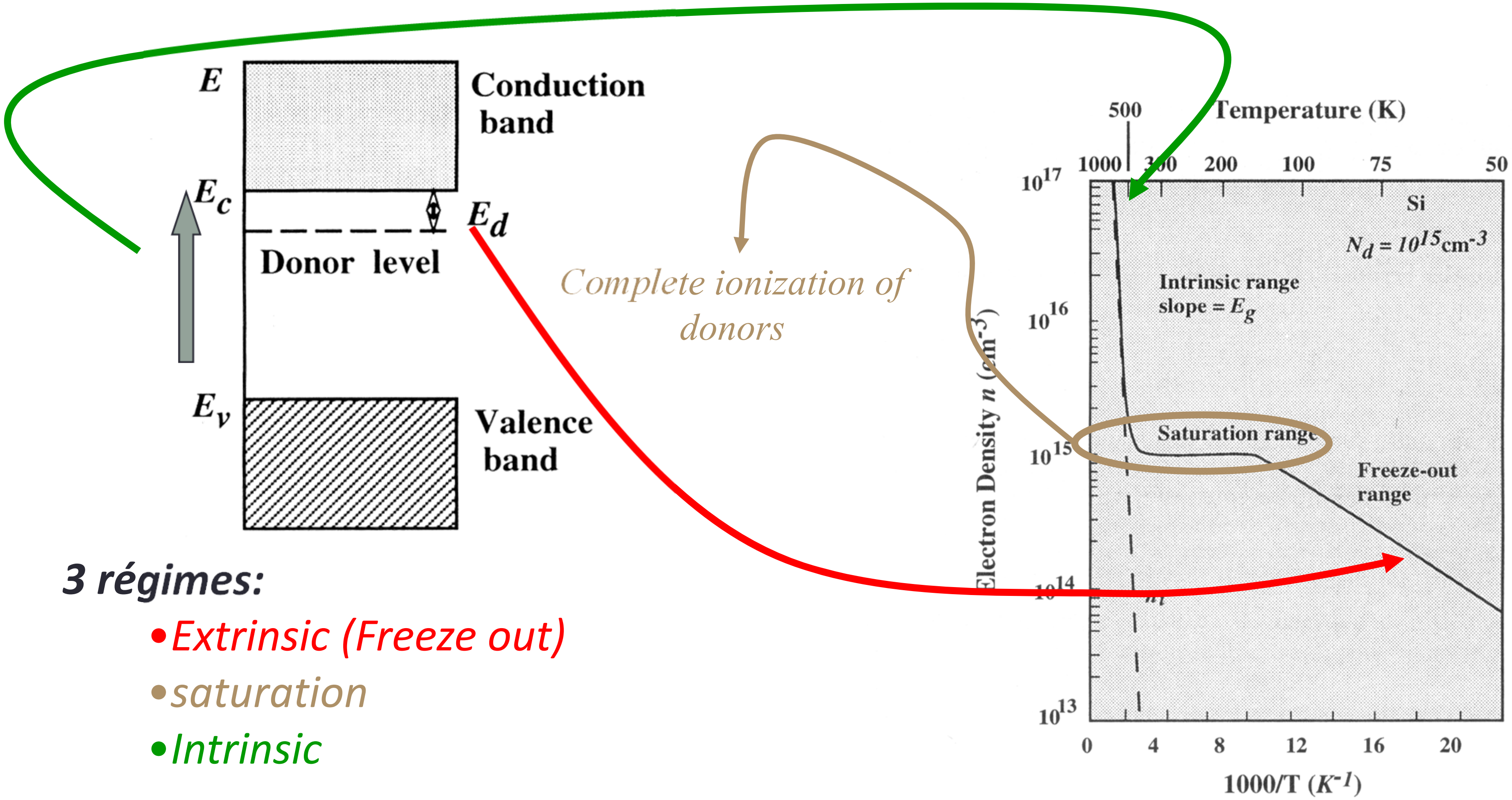


- « High » Température

  intrinsic



Carrier density versus temperature



3 régimes:

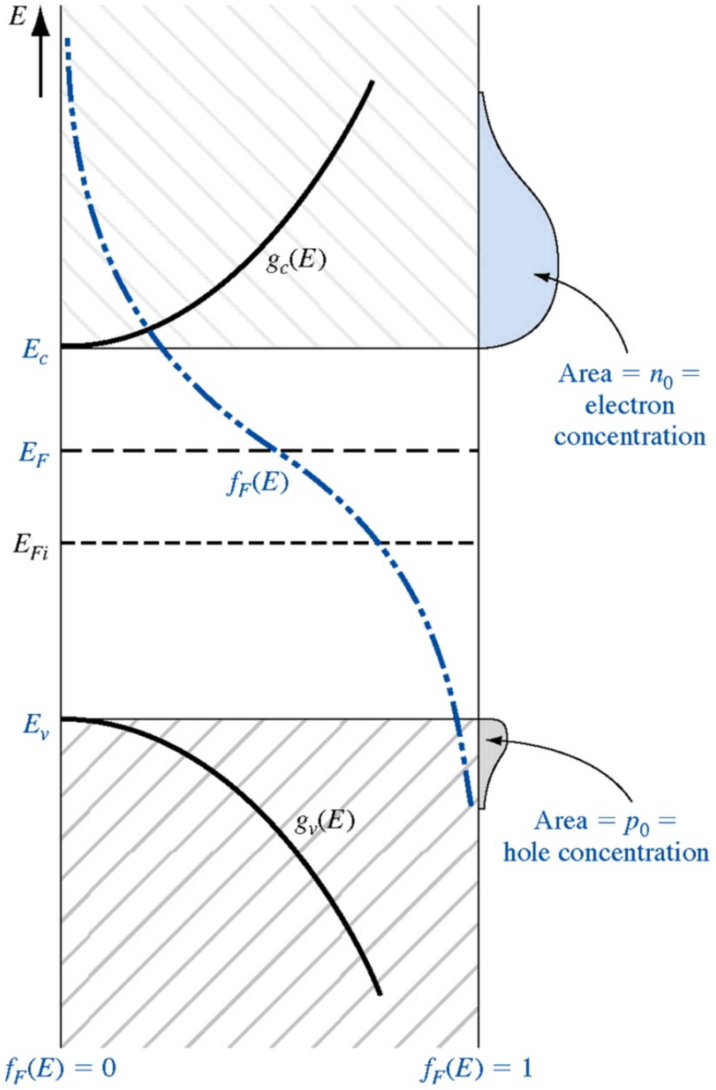
- *Extrinsic (Freeze out)*
- *saturation*
- *Intrinsic*

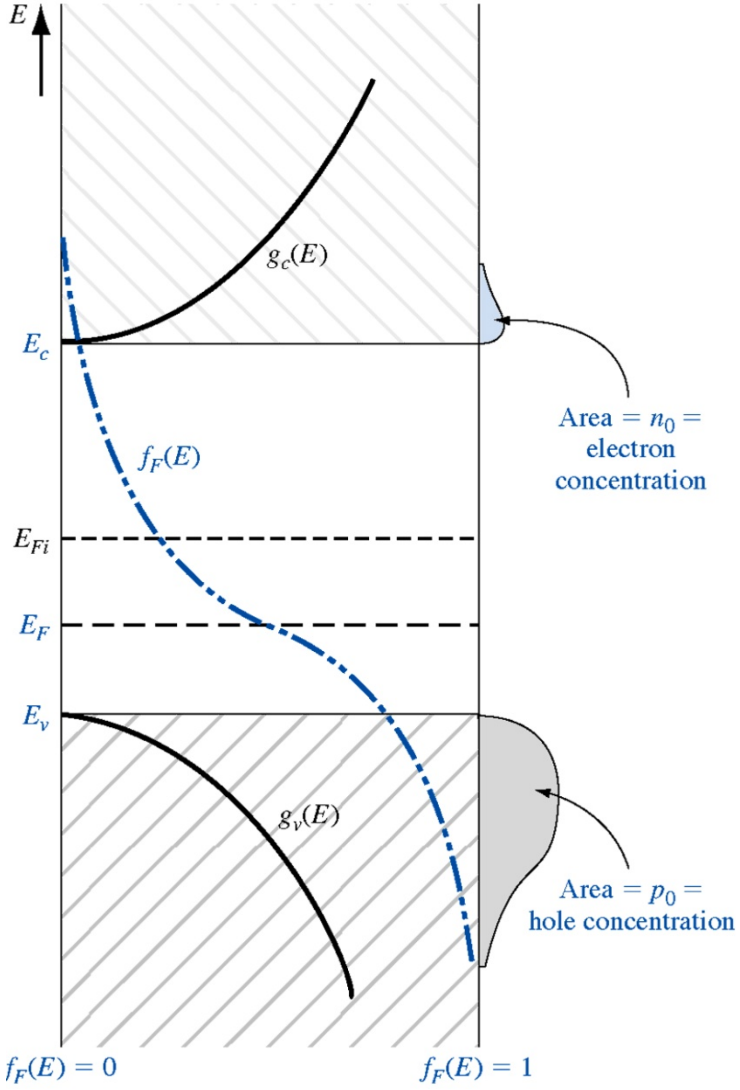
Carriers distribution at equilibrium

$$n_0 = N_c \exp\left[-\frac{(E_c - E_f)}{kT}\right] = N_c \exp\left[-\frac{(E_c - E_{fi}) - (E_f - E_{fi})}{kT}\right]$$

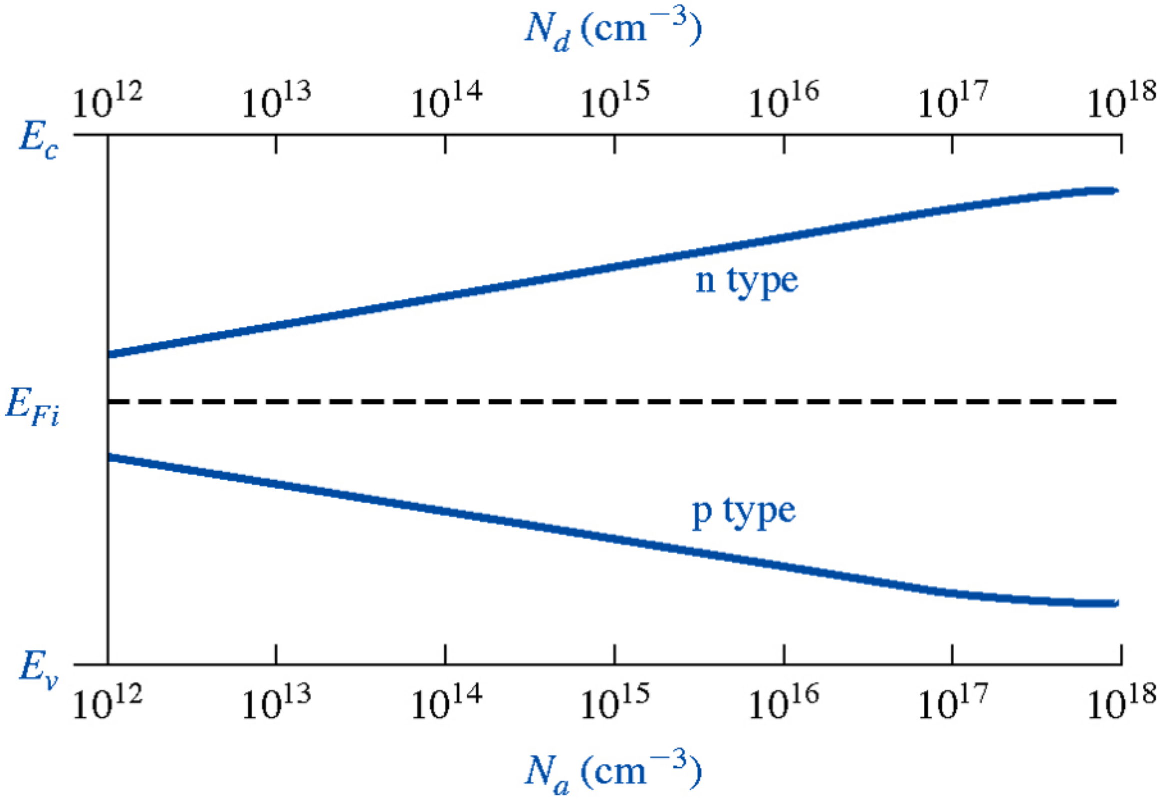
$$n_0 = N_c \exp\left[-\frac{(E_c - E_{fi})}{kT}\right] \exp\left[-\frac{(E_{fi} - E_f)}{kT}\right]$$

Fermi level in intrinsic SC

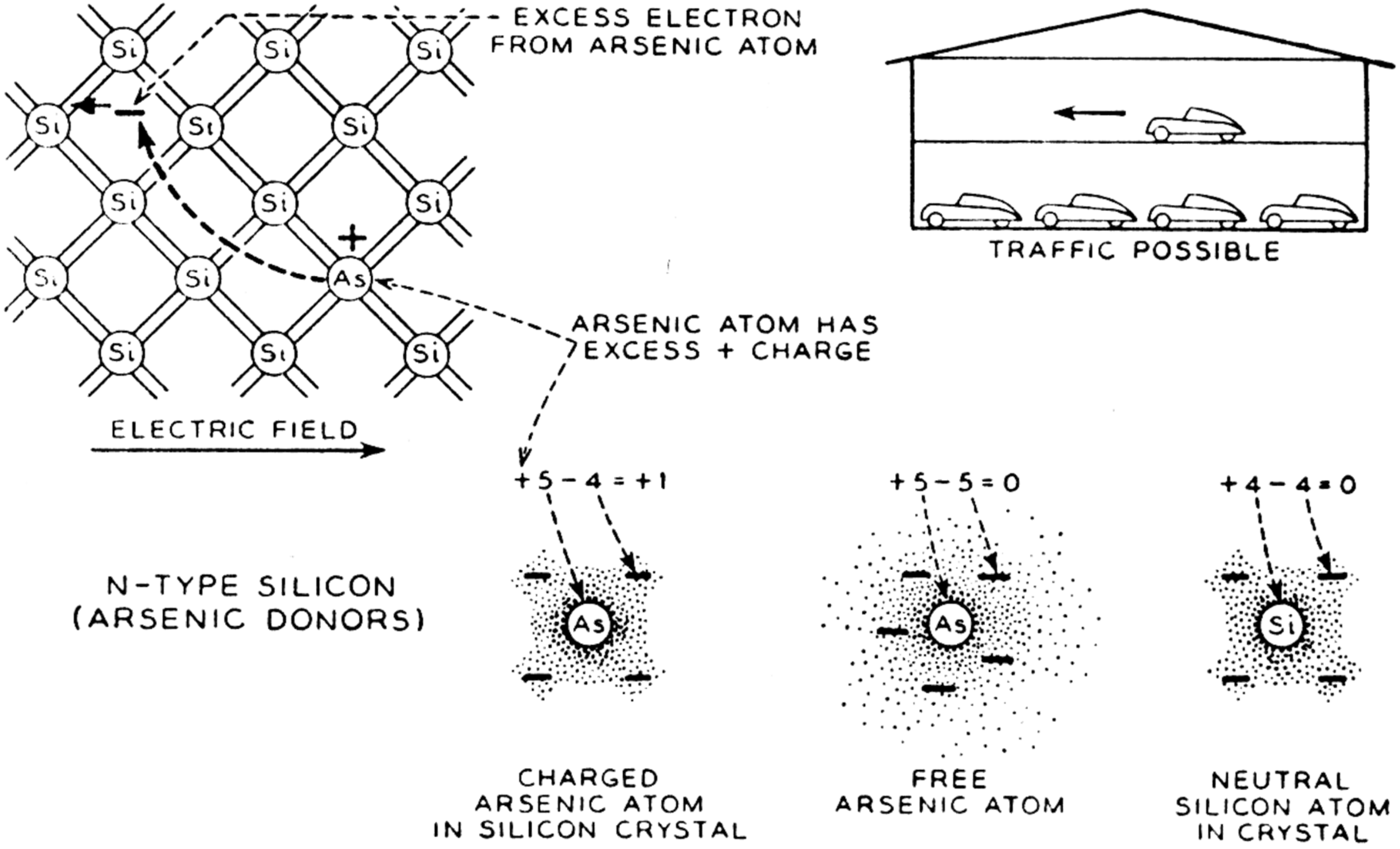




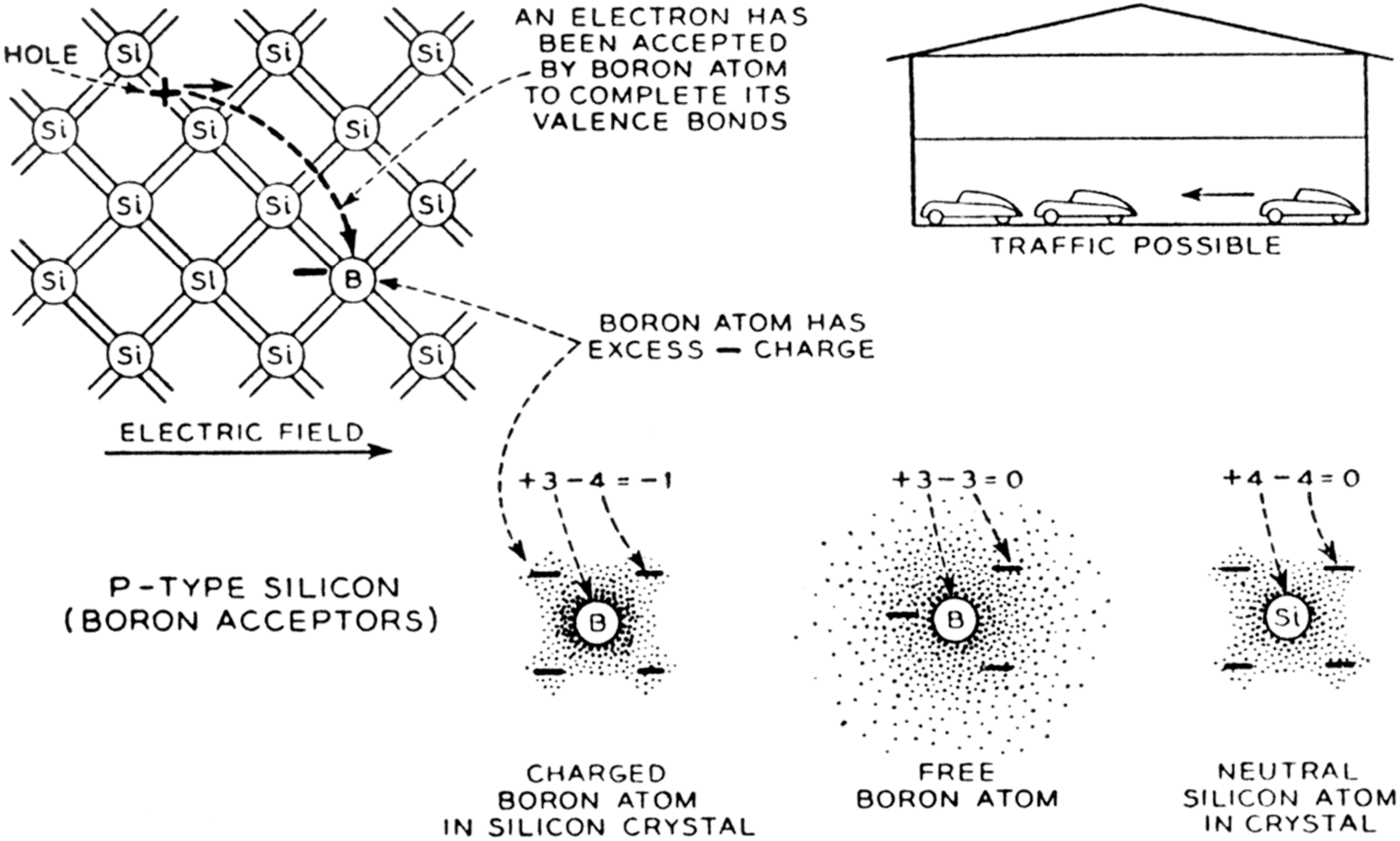
Fermi level in intrinsic SC



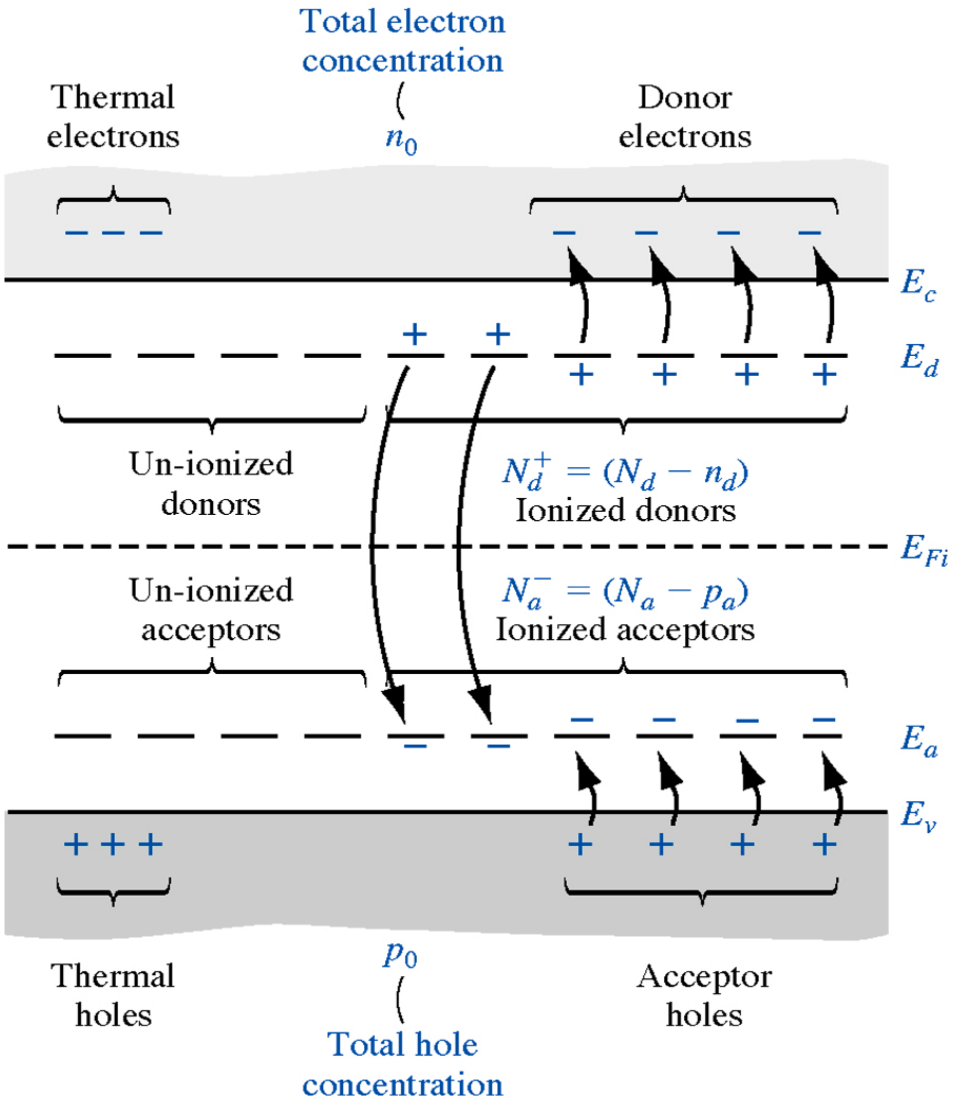
SC doping: *n type*



SC doping: *p type*



h^+ and e^- concentration at equilibrium



If there are donors and acceptors, it is a bit more complicated!

h$^+$ and e$^-$ concentration at equilibrium

- *Neutralité électrique:*

$$n_0 + N_A^- = p_0 + N_D^+$$

- *Ionisation totale:*

$$n_0 + N_A = p_0 + N_D \quad \text{avec} \quad p_0 = {n_i^2}/{n_0}$$

- *Soit:*

$$n_0^2 - (N_D - N_A)n_0 - n_i^2 = 0$$

- *On obtient:*

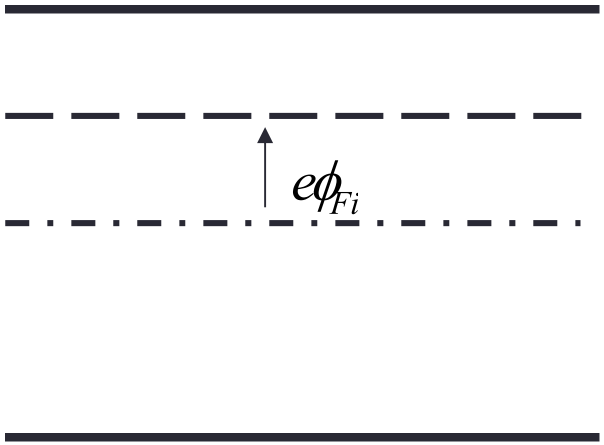
$$\boxed{n_0 = \frac{(N_D - N_A)}{2} + \sqrt{\frac{(N_D - N_A)^2}{4} + n_i^2}}$$

$E_f - E_{fi}$ difference

- Instead of expressing Ef according to Nc and Nv, we can write :

$$E_f - E_i = kT \ln\left(\frac{N_d}{n_i}\right)$$

n type



$$E_i - E_f = kT \ln\left(\frac{N_a}{n_i}\right)$$

p type

$E_f - E_{fi}$ difference

- We can then express the density of electrons and holes at equilibrium by :

$$n = n_i e^{(E_F - E_{Fi})/kT} = n_i e^{e\phi_{Fi}/kT}$$

$$p = n_i e^{-(E_F - E_{Fi})/kT} = n_i e^{-e\phi_{Fi}/kT}$$

Boltzmann approximation

with:

$$e\phi_{Fi} = E_F - E_{Fi} > 0$$

$$e\phi_{Fi} = E_F - E_{Fi} < 0$$

N type

P type

CHAPTER 11

Nonequilibrium semiconductor

Plan:

- Recombination and generation processes
- Currents in semiconductors
- Current density relations
- Continuity Equations
- Debye length
- Poisson's Equation
- Dielectric relaxation time constant

Recombination and generation processes

- Mass action law:
  - At equilibrium: $np = n_i^2$
  - Nonequilibrium state : onset of exces carrier generation and recombination processes
  - Carrier generation and recombination:

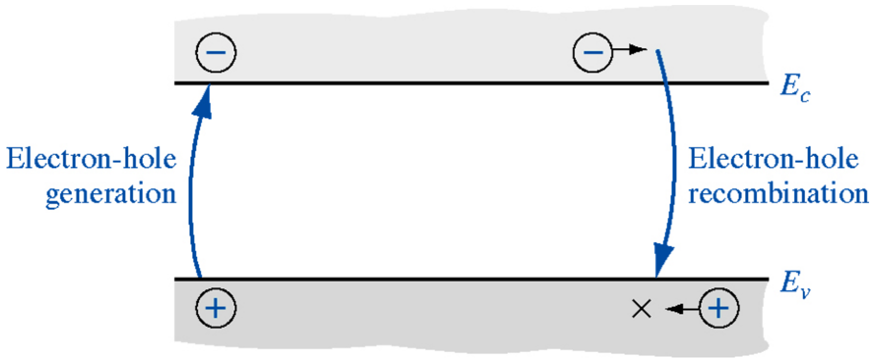
    Unity [g]=[r]=$s^{-1}cm^{-3}$
  - Net recombination rate:

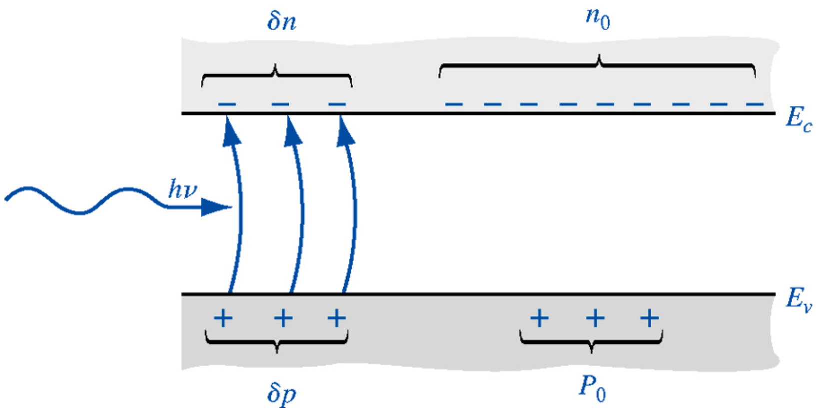
$$g' - r' = g + g_{th} - r' = \underset{\text{external}}{g} - \underset{\text{internal}}{r}$$

with

$$r = r' - g_{th}$$

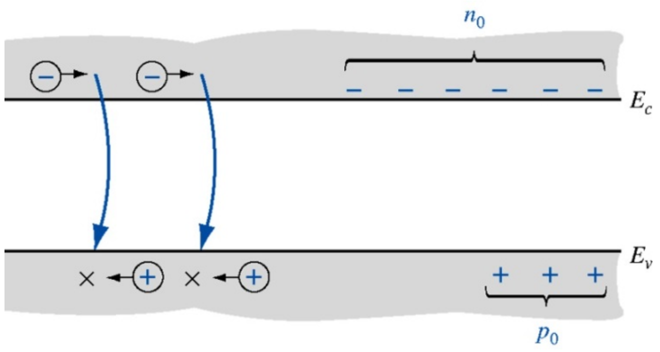
Recombination and generation processes





At equilibrium, *g* (generation rate) must be equal to r recombination rate.

If T=0K (and no light !), *g* = *r* = 0.



Recombination processes: 2 « ways » are possible (1)

- Direct Electron – hole Recombinaison
  - process is function of electrons and holes concentration:

$$r_p = \frac{\Delta p}{\tau_p} \qquad r_n = \frac{\Delta n}{\tau_n}$$

  - Example: *n type* + light excitation in low injection regime lumineuse en faible injection (ie $\Delta n = \Delta p << n_0$)

$$\boxed{p = p_0 + \Delta p} \qquad \boxed{n = n_0 + \Delta n \approx n_0}$$

  - *In low injection regime, majority caririer density is not modified.*

Recombination processes: 2 « ways » are possible (1)

- Recombination assisted by trap:
  - In general, traps are localized in the mid gap
  - Recombination can be expressed as:

$$r = \frac{1}{\tau_m} \frac{np - n_i^2}{2n_i + p + n}$$

Shockley-Read relation

where τ_m is characteristic of the trap

- If the both processes are present:

$$\frac{1}{\tau} = \frac{1}{\tau_m} + \frac{1}{\tau_{n(p)}}$$

Recombination processes: 2 « ways » are possible (3)

- If intrinsic (or low doping level) semiconductor: we apply Shockley-Read relation
- If doped semiconductor (for ex n type):

$$r_p = \frac{\Delta p}{\tau} \qquad \text{with} \qquad \frac{1}{\tau} = \frac{1}{\tau_m} + \frac{1}{\tau_p}$$

- If region with no carrier (example: space charge region)

$$r = \frac{1}{\tau_m}\,\frac{\cancel{n}p - n_i^2}{2n_i + \cancel{p} + \cancel{n}}$$

$$r = -\frac{n_i}{2\tau_m} < 0$$

Net generation rate. Charge carriers are created

Light excitation

P type

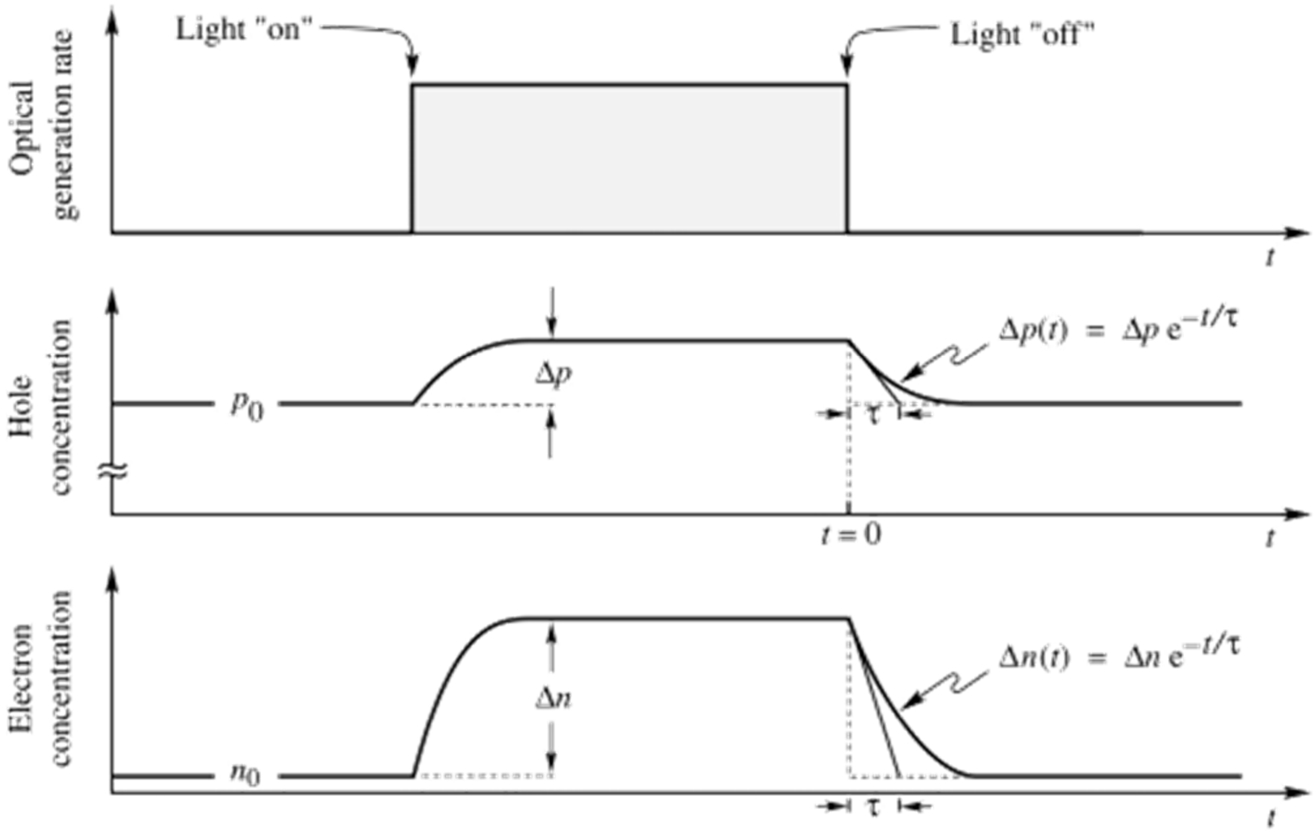


Fig. 1.2. Carrier concentration as a function of time before, during, and after an optical excitation pulse. The semiconductor is assumed to be p-type and thus it is $p_0 >> n_0$. Electrons and holes are generated in pairs, thus $\Delta p = \Delta n$. Under low-level excitation shown here, it is $\Delta n << p_0$. In most practical cases the equilibrium minority carrier concentration is extremely small so that $n_0 << \Delta n$.

radiative and nonradiative recombination

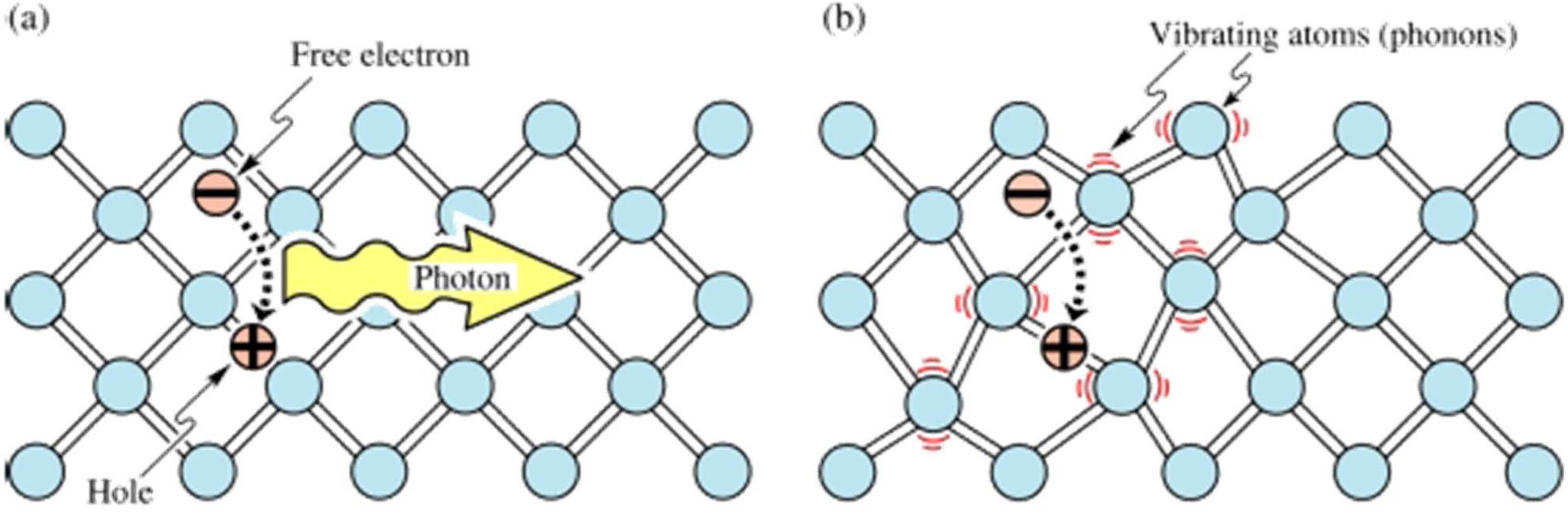


Fig. 1.5. (a) Radiative recombination of an electron-hole pair accompanied by the emission of a photon with energy $h\nu \approx E_g$. (b) In non-radiative recombination events, the energy released during the electron-hole recombination is converted to phonons (adopted from Shockley, 1950).

Surface effects

Nonradiative recombination at surfaces

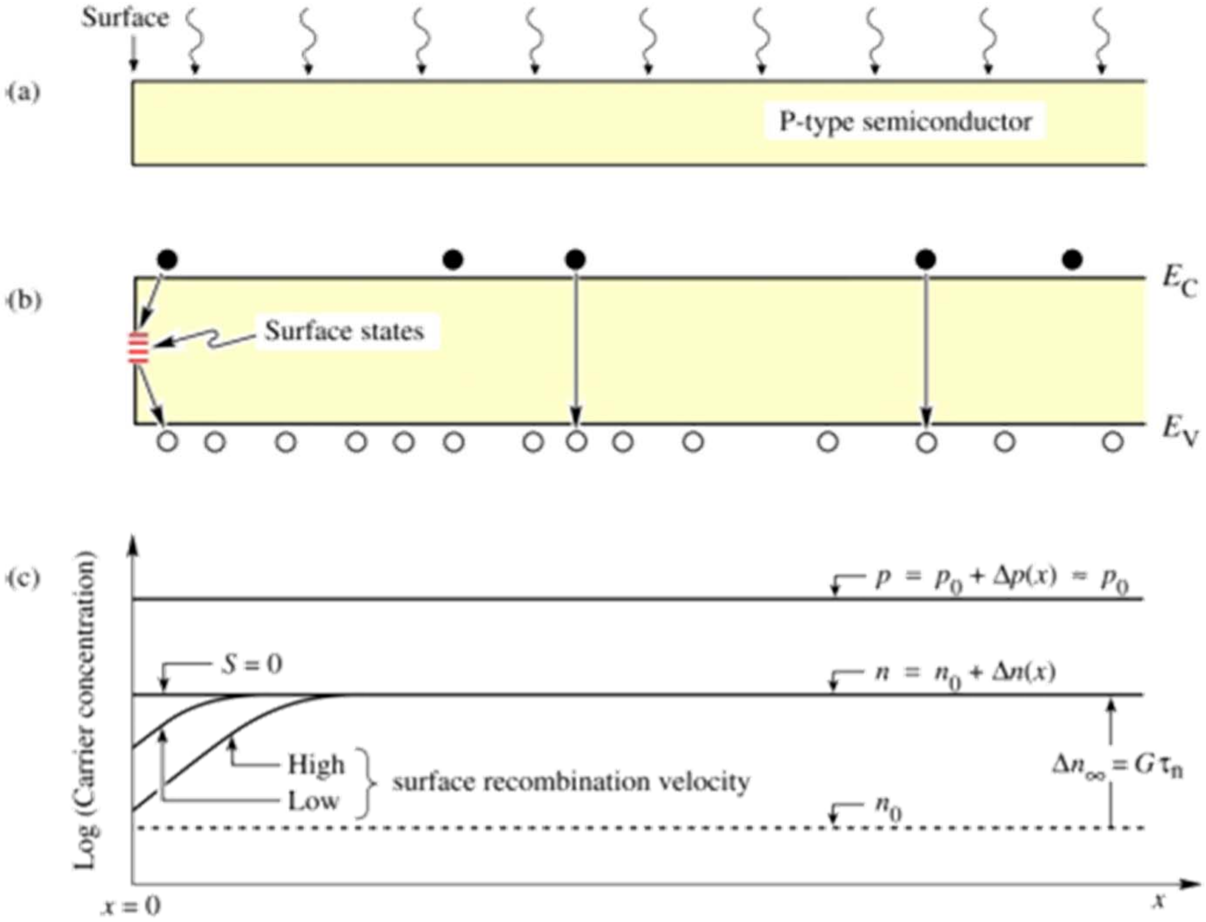


Fig. 1.9. (a) Illuminated p-type semiconductor, (b) band diagram, and (c) minority and majority carrier concentration near the surface assuming unifom carrier generation due to illumination. The excess carrier concentrations are Δn and Δp.

Currents in semiconductor

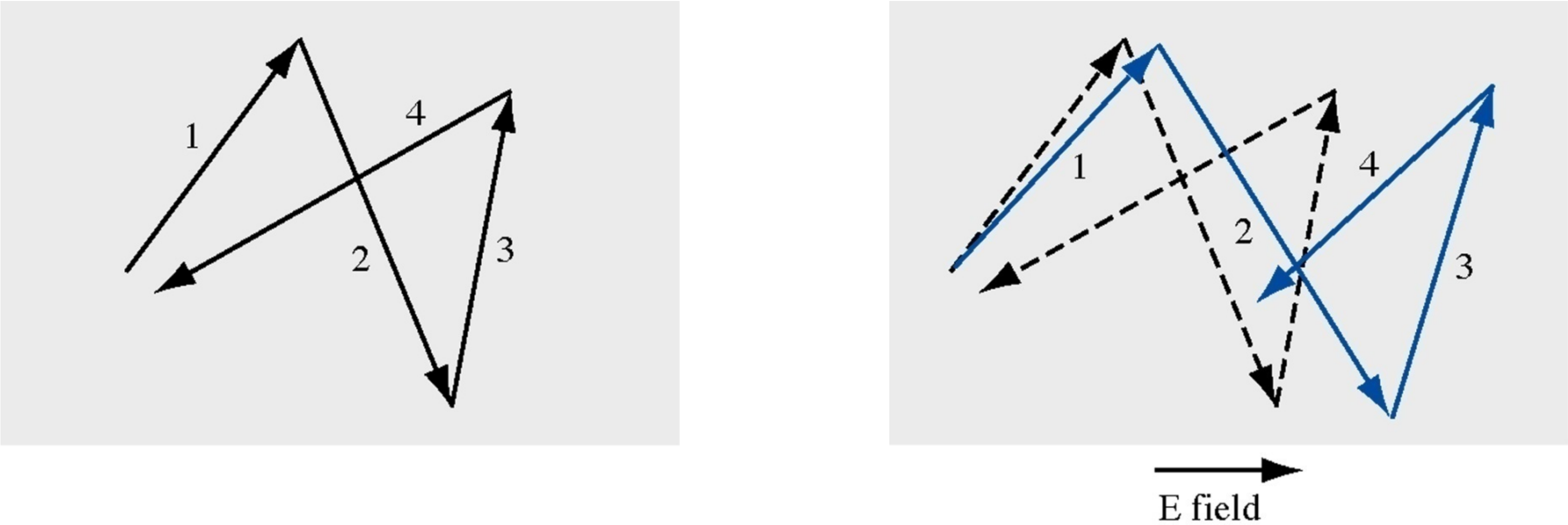
- Drift current : an electric field E is present/applied
  - If E=0, electrons velocity = thermal velocity (10^7 cm/s) but ***average velocity*** is zero due to scattering with atoms and impureties.
  - mean free path:

$$l = vth.\tau \approx 100\,\overset{o}{\mathrm{A}}$$

  - Mean time between collisions

$$\tau \approx 0.1 ps$$

drift velocity



Ramdom behavior of a hole without and with an electric field

Drift current

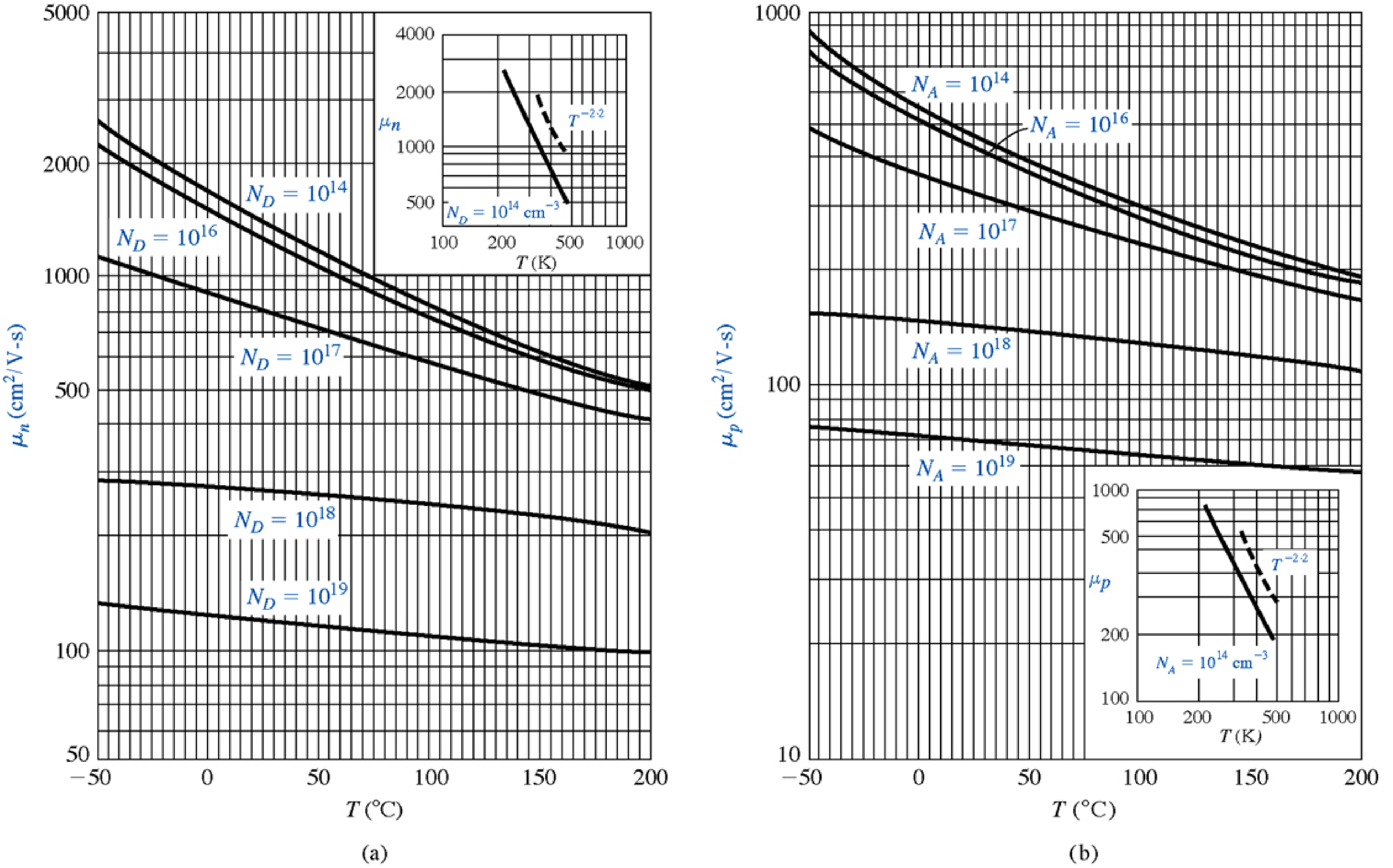
- Drift current:
  - Between two collisions, electrons are uniformly accelerated
  - Acceleration: $$\gamma = -qE/m^*$$
  - velocity: $$v = -qE\tau/m^* = \pm\mu E$$
  - Mobility: $$\mu = \left|q\tau/m^*\right|$$

Si : 1500 cm^2/Vs
GaAs: 8500 cm^2/Vs
$In_{0.53}Ga_{0.47}As$:11000 cm^2/Vs

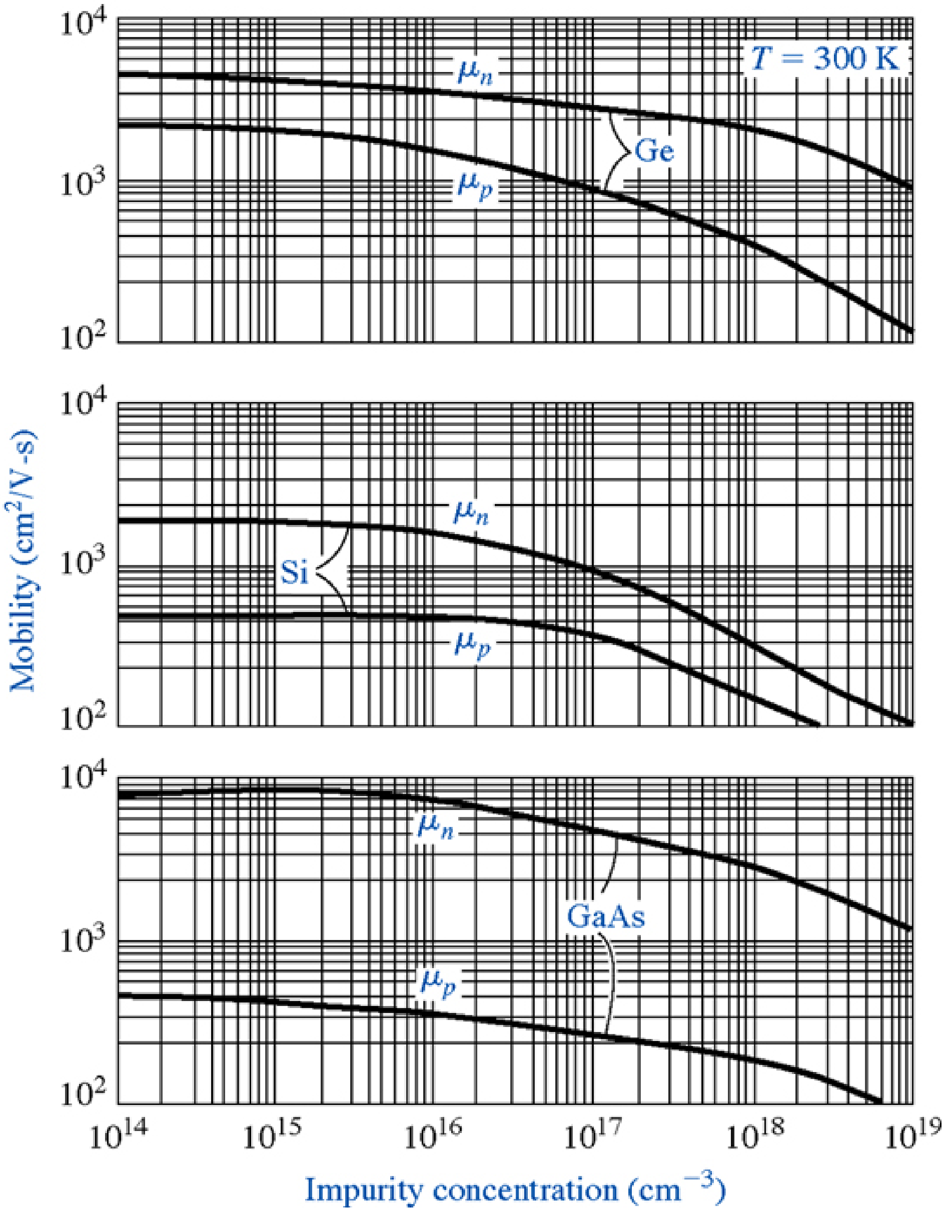
Drift current

- Drift current density:
  - For electrons: $\boxed{\vec{J}_{cn} = -ne\vec{v}_n = ne\mu_n\vec{E}}$
  - For the holes: $\boxed{\vec{J}_{cp} = +pe\vec{v}_p = pe\mu_p\vec{E}}$
  - global: $\boxed{\vec{J}_{ctotal} = \vec{J}_n + \vec{J}_p = (ne\mu_n + pe\mu_p)\vec{E}}$

Mobility versus temperature



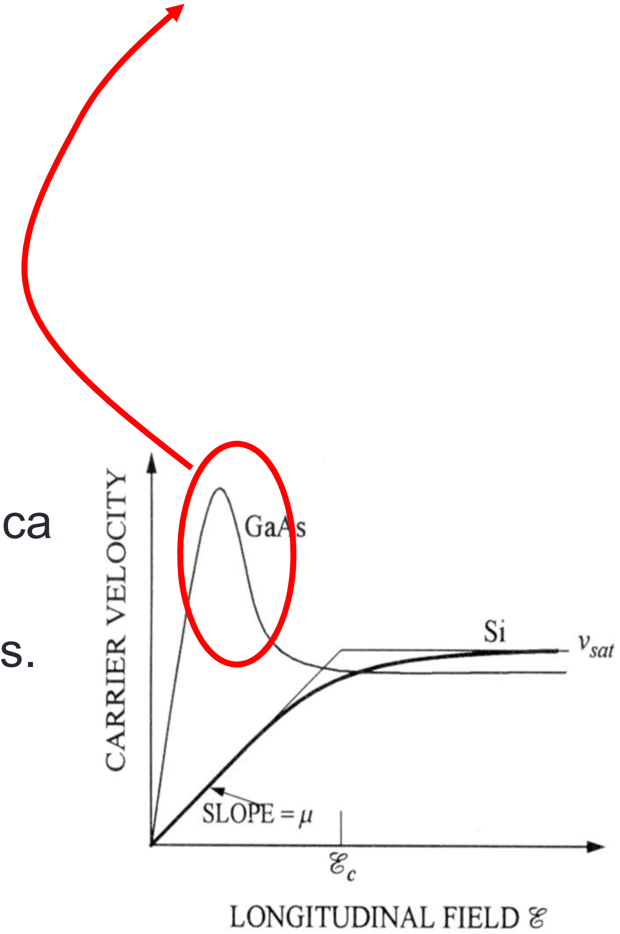
Mobility versus doping concentration



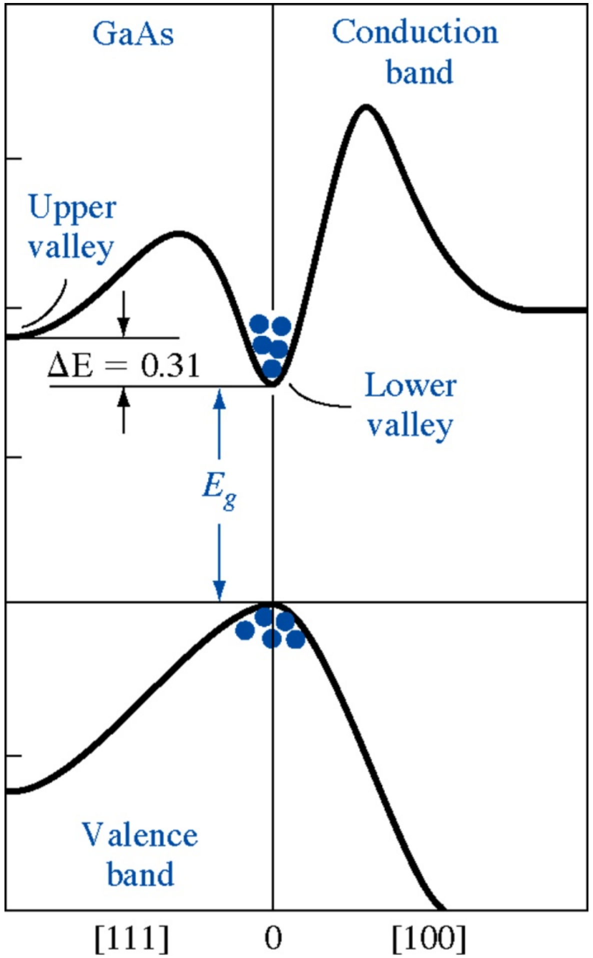
Saturation velocity

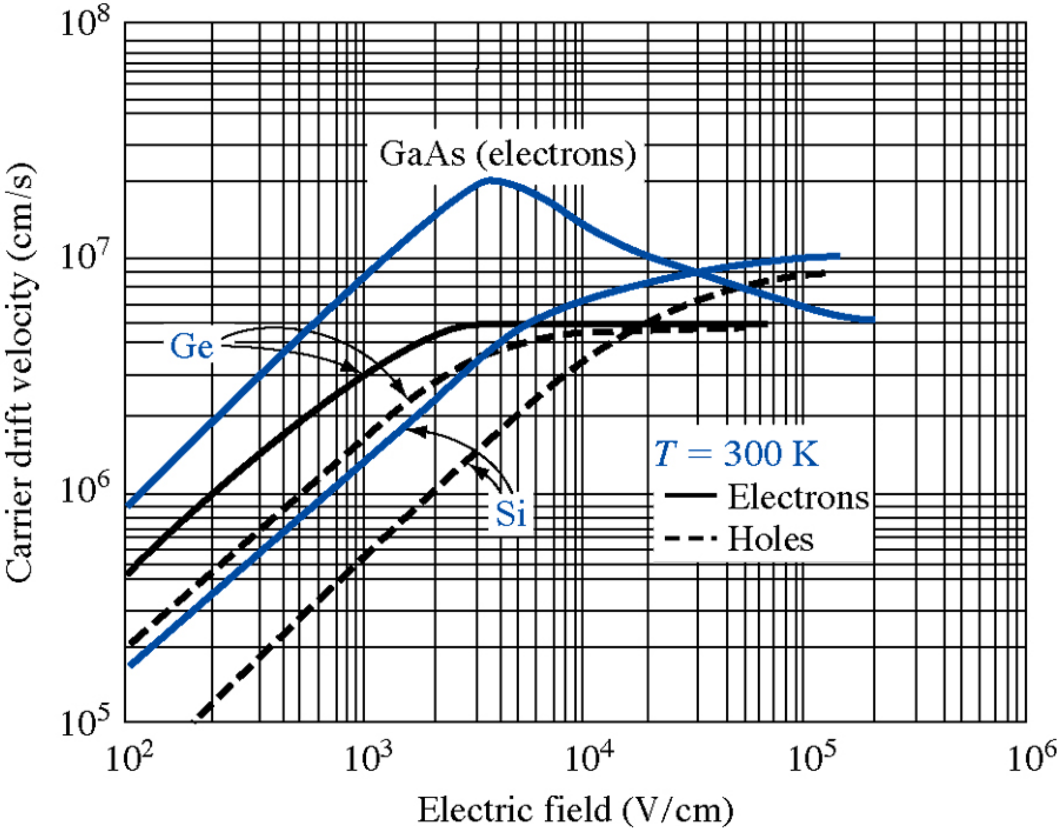
- saturation velocity of electrons
  - Linear relationship velocity – electric field only valid for:
    - Low electric field
    - Carrier in equilibrium with the lattice
  - If not:
    - velocity saturation for electric field above the critica field
    - velocity overshoot for multi-valley semiconductors.
    - Balistic regime: for devices with low dimension (below mean free path (0.1µm))

(« *overshoot* »)



Overshoot for multivaley semiconductors





Currents in semiconductors

- Diffusion current:
  - Origin: electrons (or holes) density gradient
  - Diffusion from a region from high concentration toward a region of low concentration.
  - 1st law of Fick:

$$n_D^x = -D_n \frac{dn}{dx}$$

Number of electrons which diffuse by time unit and volume unit (flow)

$$p_D^x = -D_p \frac{dp}{dx}$$

Number of holes which diffuse by time unit and volume unit (flow)

Currents in semiconductors

- Diffusion current : we sum up electrons and holes contribution:

$$J_{diff} = e(-n_D^x + p_D^x) = eD_n \frac{dn}{dx} - eD_p \frac{dp}{dx}$$

  - Electron diffusion coefficient or constant

$$\left\lfloor D_{n,p} \right\rfloor = cm^2 / s$$

Currents in semiconductors

- Total current density : we have 4 possible independant current:

$$J_T = J_{cond} + J_{diff} = J_n + J_p$$

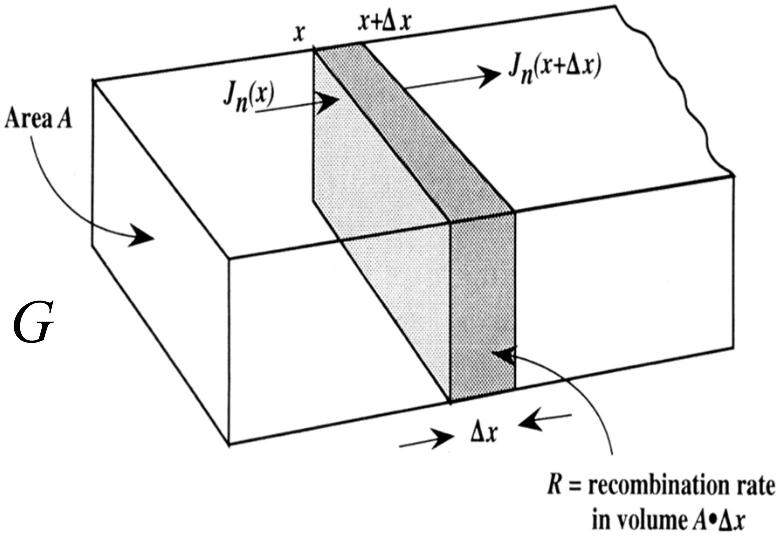
$$J_T = (ne\mu_n + pe\mu_p)E + e(D_n \frac{dn}{dx} - D_p \frac{dp}{dx})$$

- D and μ express the ability of carriers to move. There is a relationship between them : it’s the *Einstein relation*:

$$\frac{D}{\mu} = \frac{kT}{e}$$

Continuity equation – diffusion length

- G and R alter the distribution of carriers and so the current.



$$A\Delta x\frac{dn(x,t)}{dt}=A\left[\frac{J_n(x+\Delta x)}{e}-\frac{J_n(x)}{e}\right]-R+G$$

$$A\Delta x\frac{dn(x,t)}{dt}\cong A\frac{dJ_n(x)}{dx}\frac{\Delta x}{e}-R+G$$

- We obtain the continuity equations for electrons and holes:

$$\boxed{\frac{dn(x,t)}{dt}=\frac{1}{e}\frac{dJ_n}{dx}-r_n+g_n}$$

$$\boxed{\frac{dp(x,t)}{dt}=-\frac{1}{e}\frac{dJ_p}{dx}-r_p+g_p}$$

Continuity equation – diffusion length

- *Example:* case where the current is *exclusively due to a diffusion process:*

$$J_n(diff) = eD_n \frac{dn}{dx}$$

$$J_p(diff) = -eD_p \frac{dp}{dx}$$

$$\Longrightarrow$$

$$\frac{dn}{dt} = D_n \frac{d^2 n}{dx^2} - \frac{n - n_0}{\tau_n}$$

$$\frac{dp}{dt} = D_p \frac{d^2 p}{dx^2} - \frac{p - p_0}{\tau_p}$$

Continuity equation – diffusion length

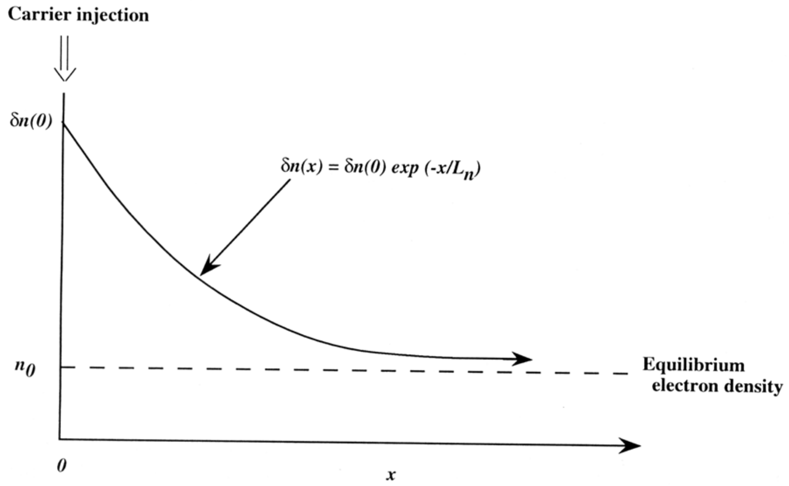
- In steady state, the time derivatives are zero:

$$\frac{d^2(n-n_0)}{dx^2} = \frac{n-n_0}{D_n\tau_n} = \frac{n-n_0}{L_n^2}$$

$$\frac{d^2(p-p_0)}{dx^2} = \frac{p-p_0}{D_p\tau_p} = \frac{p-p_0}{L_p^2}$$

$$\boxed{L_n = \sqrt{D_n\tau_n}} \qquad \boxed{L_p = \sqrt{D_p\tau_p}}$$

$$\boxed{\Delta n(x) = (n(x)-n_0) = \Delta n(0)e^{-x/L_n}}$$



- *Diffusion length* : represents the mean distance an electron (a hole) can travel before it recombines with a hole (an electron)
- L_n or L_p >> VLSI devices

Poisson's equation

- Comes from the first Maxwell equation. It etablishes a relation between electric potential (V(x)) and charge carrier density (ρ(x)):

$$\frac{d^2V}{dx^2} = -\frac{dE}{dx} = -\frac{\rho(x)}{\varepsilon_{sc}}$$

- In the SC, two types of charges (fixes and mobiles):

$$\frac{d^2V}{dx^2} = -\frac{e}{\varepsilon_{sc}}\left[\underbrace{p(x) - n(x)}_{\substack{\textit{Mobile Charges}\\ \textit{(electrons and holes)}}} + \underbrace{N_D^+(x) - N_A^-(x)}_{\substack{\textit{Fixe Charges}\\ \textit{(ionised dopants)}}}\right]$$

Debye length

- If we write Poisson's equation in an n type SC and if we express n with respect of ϕ_{Fi} :

$$\frac{d^2\Phi_{Fi}}{dx^2} = -\frac{e}{\varepsilon_{sc}}\left[N_d(x) - n_i e^{e\Phi_{Fi}/kT}\right]$$

- If $N_d(x) \Rightarrow N_d + \Delta N_d(x)$, then Φ_{Fi} is modified by a quantity $\Delta\Phi_{Fi}$

If we remark that : $V(x) = \Phi_{Fi} + cte$

$$\frac{d^2\Delta\phi_{Fi}}{dx^2} - \frac{e^2 N_d}{\varepsilon_{sc} kT}\Delta\phi_{Fi} = -\frac{e}{\varepsilon_{sc}}\Delta N_d(x)$$

Debye length

- Physical meaning ?
  - Solution of the differential equation :

$$\Delta\phi_{Fi} = A\exp - \frac{x}{L_D} \qquad \text{avec} \qquad L_D = \sqrt{\frac{\varepsilon_{sc} kT}{e^2 N_D}}$$

  - The energy bands can’t vary abruptly (and in the same maner the carrier density), but need few L_D (if N_d=10^{16} cm^{-3}, L_D=0.04µm). In this region, an electric field appears.

Dielectric relaxation time constant

- Comment évolue dans le temps la densité de *porteurs majoritaires* ?
  - Équation de continuité (R et G négligés):

$$\frac{\partial n}{\partial t} = \frac{1}{e}\frac{\partial J_n}{\partial x} \quad \text{or} \quad J_n = \sigma E = E / \rho_n \quad \text{et} \quad \frac{\partial E}{\partial x} = -en/\varepsilon_{sc}$$

d'où

$$\frac{\partial n}{\partial t} = -\frac{n}{\rho_n \varepsilon_{sc}}$$

Solution: $n(t) \propto \exp(-t/\rho_n \varepsilon_{sc})$

$$\tau = \rho_n \varepsilon_{sc}$$

Temps de relaxation diélectrique (10^{-12} s)

CHAP 12

The PN junction diode

PN Homojunction

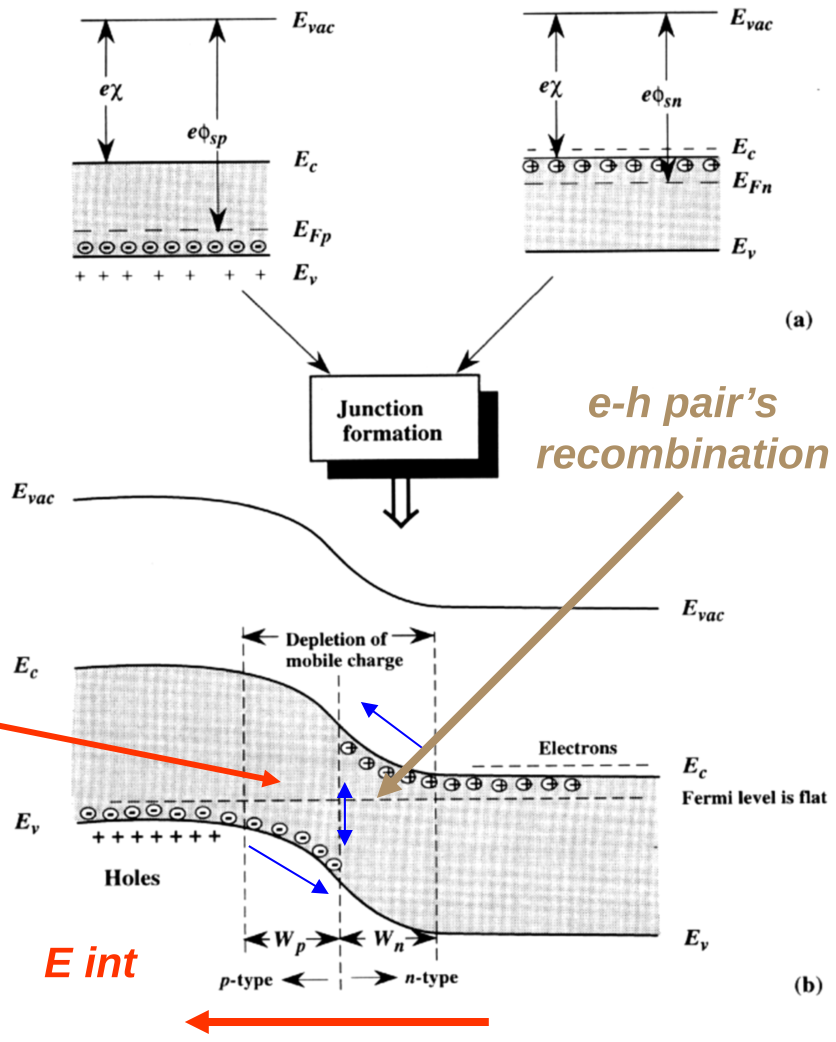
- Non linear device
- rectifier devices (composants redresseur)
- 2 devices reach the same results:
    - PN Junction(this chapter)
    - Schottky barrier or Metal / SC contact (next chapter)

The Junction’s formation mechanism

- PN Junction at equilibrium

1st Step: diffusion mechanism

2nd Step: built in Electric Field appears⇔ compensates diffusion forces



e-h pair’s recombination

E int

Flat Fermi level:
No current / thermal equilibrium

« built in potential V_{Bi} »

- Definition : Potential drop between N and P regions

$$V_{bi} = V_N - V_P$$

Holes current equation:

$$J_P(x) = e\left[\mu_P p(x)E(x) - D_p \frac{dp(x)}{dx}\right] = 0$$

or

$$\frac{\mu_p}{D_p}E(x) = \frac{1}{p(x)}\frac{dp(x)}{dx}$$

or

$$\frac{-e}{kT}\frac{dV(x)}{dx} = \frac{1}{p(x)}\frac{dp(x)}{dx}$$

Integrating from P to N region:

$$V_{bi} = \frac{kT}{e}\ln\left(\frac{p_p}{p_n}\right)$$

finally:

$$V_D = V_{bi} = \frac{kT}{e}\ln\left(\frac{N_A N_D}{n_i^2}\right)$$

•Field, potential and Space Charge width(1)

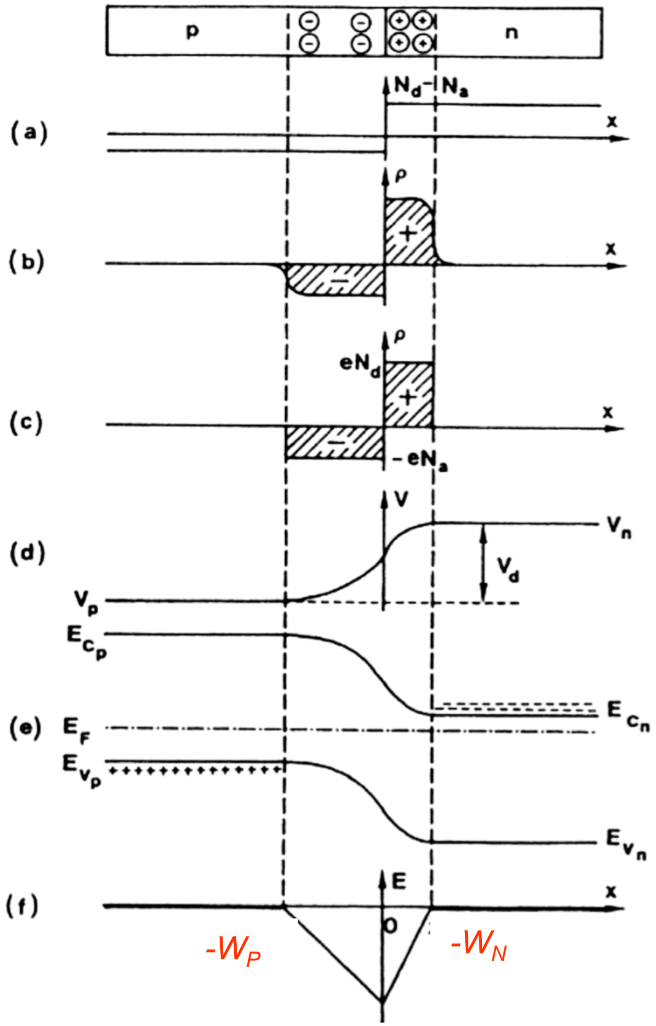
- *Poisson's equation:*

$$\frac{d^2V(x)}{dx^2} = -\frac{\rho(x)}{\varepsilon_{sc}}$$

- *In N and P region:*

$$\frac{d^2V(x)}{dx^2} = -\frac{e}{\varepsilon_{sc}} N_D \qquad 0 < x < W_N$$

$$\frac{d^2V(x)}{dx^2} = +\frac{e}{\varepsilon_{sc}} N_A \qquad -W_P < x < 0$$



•Field, potential and Space Charge width(2)

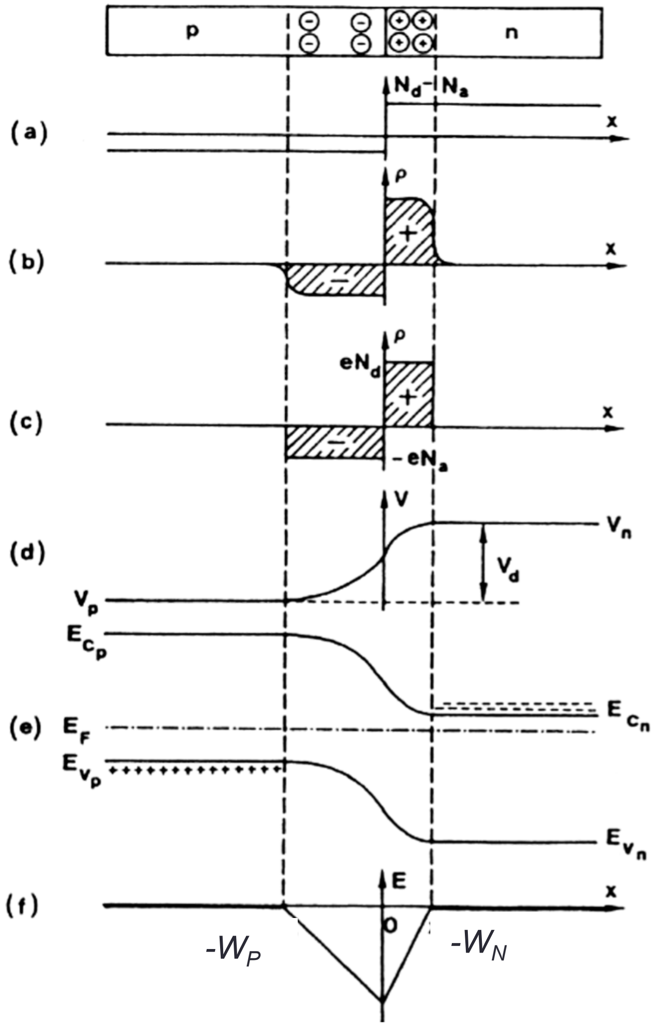
- Electric Field E(x)

$$E_n(x) = +\frac{eN_D}{\varepsilon_{sc}}(x - W_N) \qquad E_P(x) = -\frac{eN_A}{\varepsilon_{sc}}(x + W_P)$$

- Continuity of Field on x=0:

$$\boxed{N_D W_N = N_A W_P}$$

$$E_M = -\frac{eN_D W_N}{\varepsilon_{sc}} = -\frac{eN_A W_P}{\varepsilon_{sc}}$$



•Field, potential and Space Charge width(3)

- Built in potential V(x)

$$V_n(x) = -\frac{eN_D}{2\varepsilon_{sc}}(x - W_N)^2 + V_n$$

$$V_p(x) = \frac{eN_A}{2\varepsilon_{sc}}(x + W_P)^2 + V_p$$

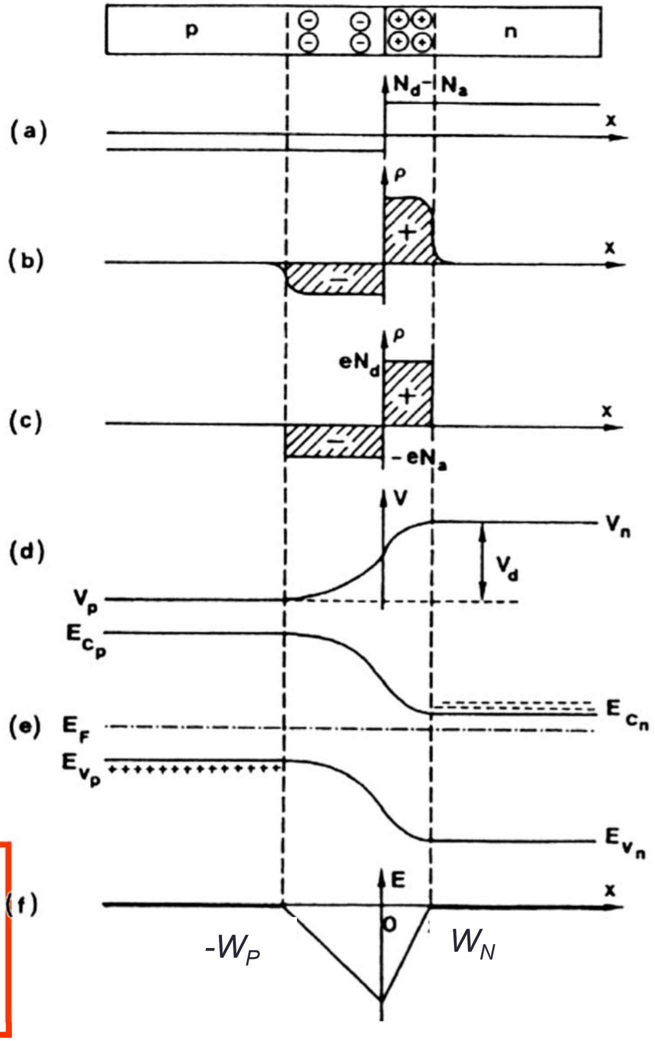
- Depletion layer (ZCE)

$$V(W_n) - V(-W_p) = V_d = \frac{eN_D W_n^2}{2\varepsilon_{sc}} + \frac{eN_A W_p^2}{2\varepsilon_{sc}}$$

$$W_p(V_d) = \sqrt{\frac{2\varepsilon_{sc}}{e}\frac{N_D}{N_A(N_A + N_D)}V_d}$$

$$W_n(V_d) = \sqrt{\frac{2\varepsilon_{sc}}{e}\frac{N_A}{N_D(N_A + N_D)}V_d}$$

$$\boxed{W(V_d) = \sqrt{\frac{2\varepsilon_{sc}}{e}\frac{N_D + N_A}{N_A N_D}V_d}}$$



WARNING: WHEN A VOLTAGE V IS APPLIED ON P SIDE, V_{BI} HAVE TO BE REPLACED BY $V_{BI} - V$

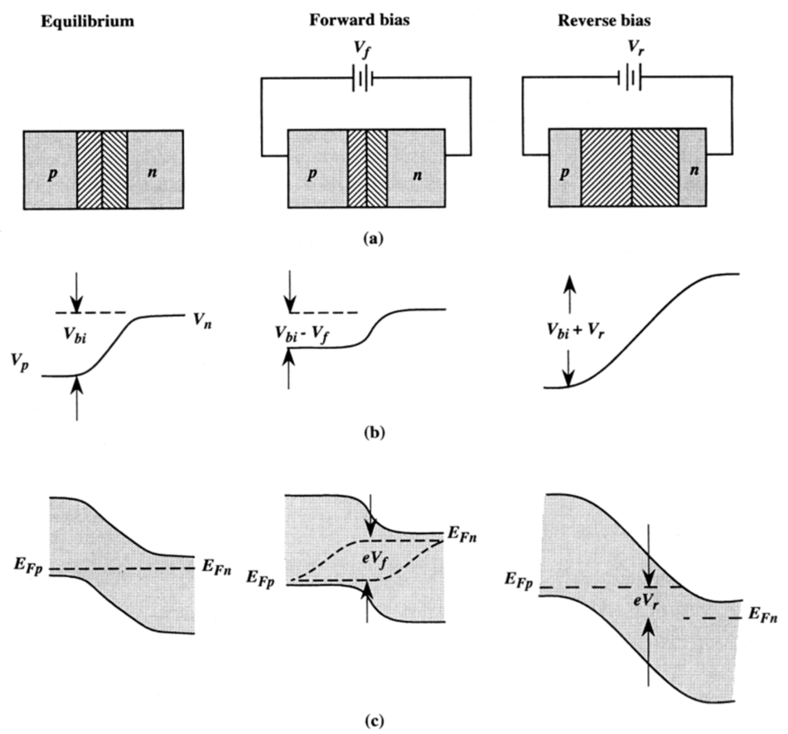
BIASED PN JUNCTION

- When a positive voltage is applied on p side, the equilibrium is destroyed and a net current can flow

- simplifying assumptions :
  - Depletion layer with no free carriers (e- and h+)
  - Low injection
  - Boltzmann’s approximation
  - Drop voltage only in depletion layer
  - No generation-recombination mechanisms present

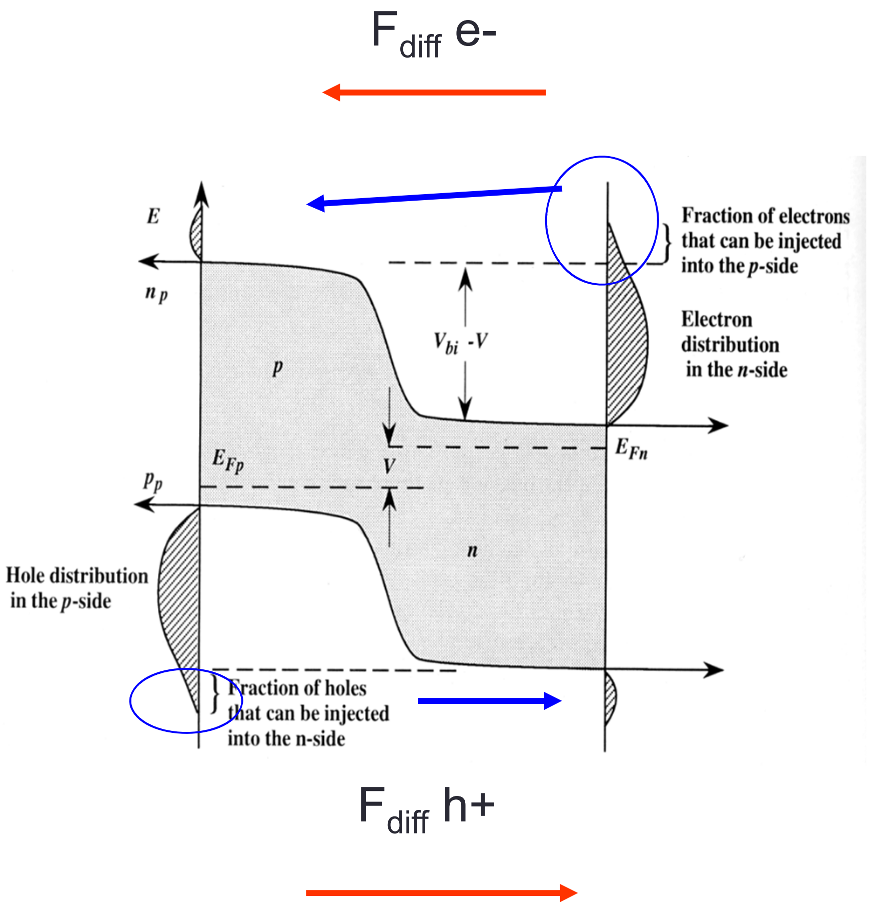
BIASED PN JUNCTION

- Foward Biasing
  - Positive voltage on P
  - lowering of built in potential
  - Diffusion mechanism dominates
  - High current

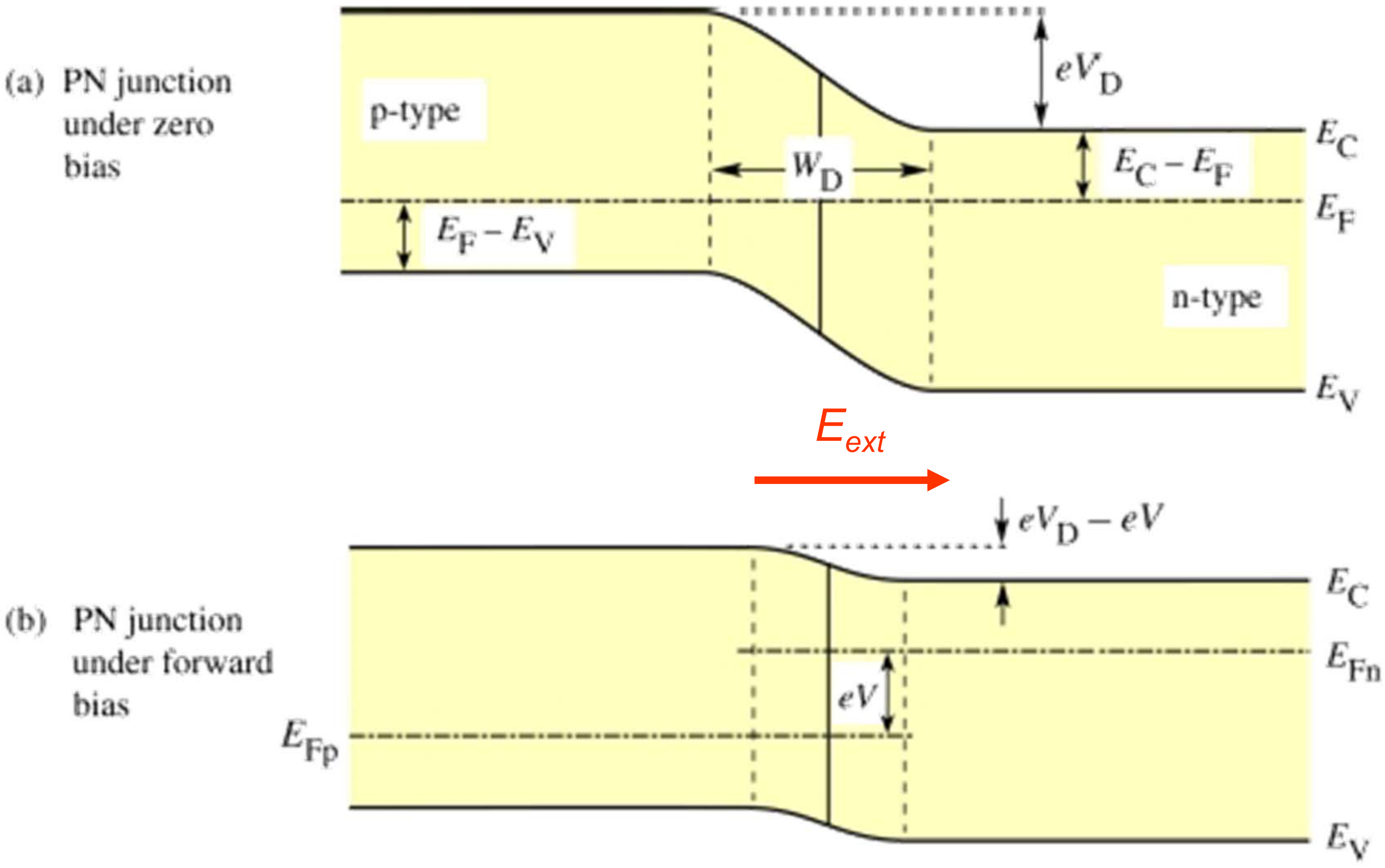


BIASED PN JUNCTION

- Forward biasing
  - Lowering of built in Field due to opposite external field
  - Electrons injected from N to P regions: minoritary carriers injection
  - High current due to full « reservoir »

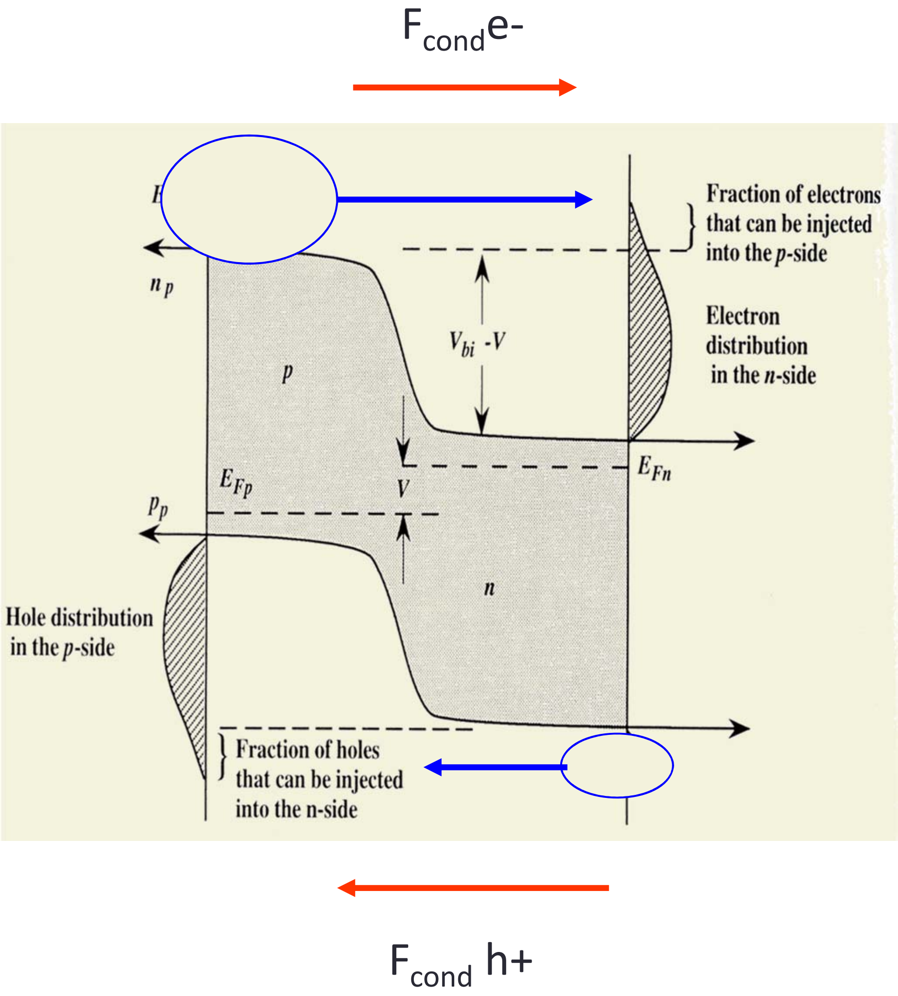


Forward Biasing



Jonction PN sous polarisation

- Reverse Biasing
  - Global Electric Field increases (External Field added to built in Field)
  - Injection of electrons from P to N and holes injection from N to P: majority carriers injection
  - Low current (leak current) due to empty « reservoir »



PN Junction under biasing

At equilibrium, null current ⇔ two components compensate between it. Taken separately, the magnitude of these components 10^4 A / cm^2 (ie 1A for typical diode) and at low injection I is of the order of few mA (max 10mA)

- ***Boltzmann's Approximation:*** *The Boltzmann approximation is to say that the resulting current being small compared with the components of this current, we consider that we are still in quasi equilibrium and therefore that the current's equation is still valid by replacing* V_{bi} *by* $V_{bi}-V_A$ *:*

$$\frac{-e}{kT}\frac{dV(x)}{dx} \enclose{circle}{\approx} \frac{1}{p(x)}\frac{dp(x)}{dx}$$

Density of carriers injected to the limits of depletion layer

- If Va=0

$$\frac{p(W_N)}{p_p} = \frac{p_n}{p_p}\exp(-\frac{eV_{bi}}{kT})$$

- If Va $\neq$ 0

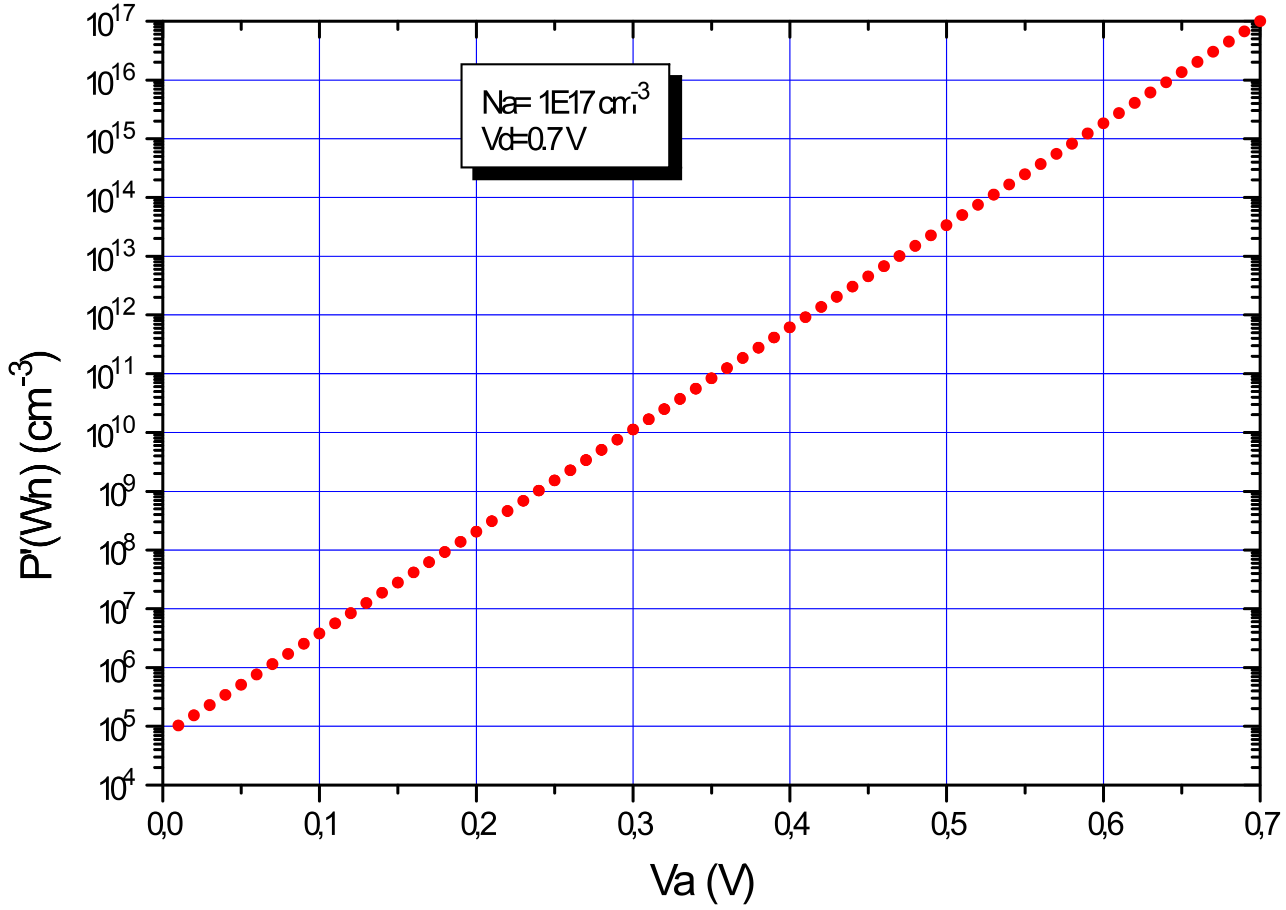
$$\frac{p'(W_N)}{p_p} = \frac{p'_n}{p_p} = \exp(-\frac{e(V_{bi}-V_A)}{kT}) = \frac{p_n}{p_p}\exp(\frac{eV_A}{kT})$$

$$p'_n = p_n \exp(\frac{eV_A}{kT}) = \frac{n_i^2}{N_D}\exp(\frac{eV_A}{kT})$$

$$n'_p = n_p \exp(\frac{eV_A}{kT}) = \frac{n_i^2}{N_A}\exp(\frac{eV_A}{kT})$$

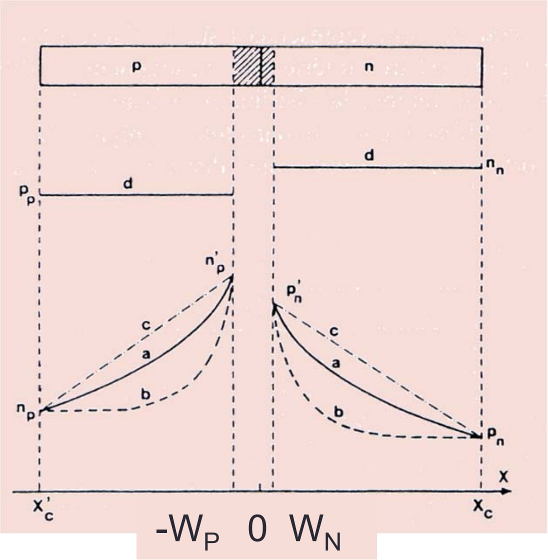
$$\boxed{n_p^{'} * p_p = p_n^{'} * n_n = n_i^2 \exp(\frac{eV_a}{kT})}$$

Holes density injected versus bias voltage V_a



Minority carriers distribution in neutral region

- Due to gradient concentration, carriers will diffuse and produce diffusion current (no electric field in neutral region !)
- Distribution is geometry dependant
- Discrimatory parameter : length diffusion $L_{Dn,p}$ of electrons and holes and neutral region widths $d_{n,p}$



Minority carriers distribution in neutral region

- *Long regions* ($d_{n,p} >> L_{p,n}$)

$$p'(x) - p_n = p_n(e^{\frac{eV_a}{kT}} - 1)e^{(W_N - x)/L_p}$$

$$n'(x) - n_p = n_p(e^{\frac{eV_a}{kT}} - 1)e^{(x+Wp)/L_n}$$

- *Short (narrow) regions* ($d_{n,p} << L_{p,n}$)

$$p'(x) - p_n = \frac{p_n}{d_n}(e^{\frac{eV_a}{kT}} - 1)(x_c - x)$$

$$n'(x) - n_p = \frac{n_p}{d_p}(e^{\frac{eV_a}{kT}} - 1)(x'_c + x)$$

- *General case*

$$p'(x) - p_n = \frac{p_n}{sh(\frac{d_n}{L_p})}(e^{\frac{eV_a}{kT}} - 1)sh\left[\frac{(x_c - x)}{L_p}\right]$$

$$n'(x) - n_p = \frac{n_p}{sh(\frac{d_p}{L_n})}(e^{\frac{eV_a}{kT}} - 1)sh\left[\frac{(x + x_c^{'})}{L_n}\right]$$

Minority currents in neutral region

Knowing minority distribution we are in position to calculate the current wich is a diffusion current (very low field in neutral region):

$$J_p(x) = -eD_p \frac{dp(x)}{dx} \qquad J_n(x) = eD_n \frac{dn(x)}{dx}$$

- Hypothesis : no G-R process in depletion layer (ZCE)

$$J(V) = J_p(-W_p) + J_n(W_p) = J_p(W_n) + J_n(-W_p)$$

- We get the classical and well known diode equation:

$$J(V) = J_S(e^{eV/kT} - 1)$$

Js is the theorical saturation current or reverse current

Minority currents in neutral region

- Short (Narrow) region

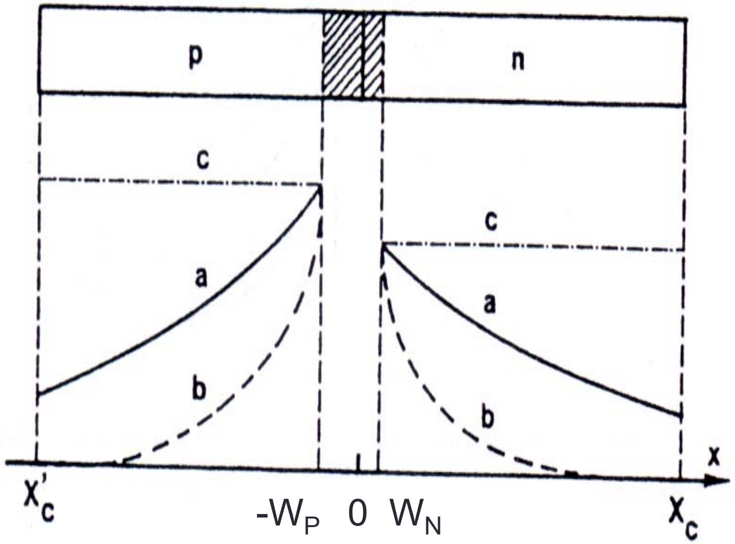
$$J_S = \frac{en_i^2 D_P}{N_D d_n} + \frac{en_i^2 D_n}{N_A d_p}$$

- Long region

$$J_S = \frac{en_i^2 D_P}{N_D L_P} + \frac{en_i^2 D_n}{N_A L_n}$$

- General case

$$J_S = \frac{en_i^2 D_P}{N_D L_P th(\frac{d_n}{L_P})} + \frac{en_i^2 D_n}{N_A L_n th(\frac{d_p}{L_n})}$$



The real diode: generation-recombinaison mechanism in depletion layer

- The model is refined ⇔ we take into account G-R process in depletion layer
- Well understood mechanism (Shockley-Read)

$$r = \frac{1}{\tau}\frac{pn - n_i^2}{2n_i + p + n}$$

- We know that $p(W_N)n(W_N) = p(W_P)n(W_P) = n_i^2 \exp(\frac{eVa}{kT})$
- If we suppose *np* constant in depleted region and *np* >> n_i^2 (in forward bias) , the rate *r* is max when *n=p,* and it can be rewritten

$$r_{\max} = \frac{n_i}{2\tau}\exp\left(\frac{eV_a}{2kT}\right)$$

The real diode: génération-recombinaison mechanism in depletion layer

- Generation-Recombinaison current in depletion layer can be expressed as:

$$J_n(W_n) - J_n(-W_p) = J_{GR} = e\int_{W_P}^{W_N} r\,dx$$

- For reverse biasing ($pn << n_i^2$), we have a negative rate ($r = -\frac{n_i}{2\tau} < 0$) . It means dans we have a net generation process

- For forward bias, r_{max}=*cte>0* and the current is due to recombinations.

The real diode: genération-recombinaison mechanism in depletion layer

- Finally GR current present in depletion layer can be expressed as:

$$J_{GR} = J_{GR}^{0}\left(\exp(\frac{eV_a}{2kT}) - 1\right) \qquad J_{GR}^{0} = \frac{en_i}{2\tau}W_T$$

- If we take into account the diffusion current, we get:

$$J(V_a) = J_S\left(\exp(\frac{eV_a}{kT}) - 1\right) + J_{GR}^{0}\left(\exp(\frac{eV_a}{2kT}) - 1\right)$$

- The expression above can be generalized by introducing Ideality factor:

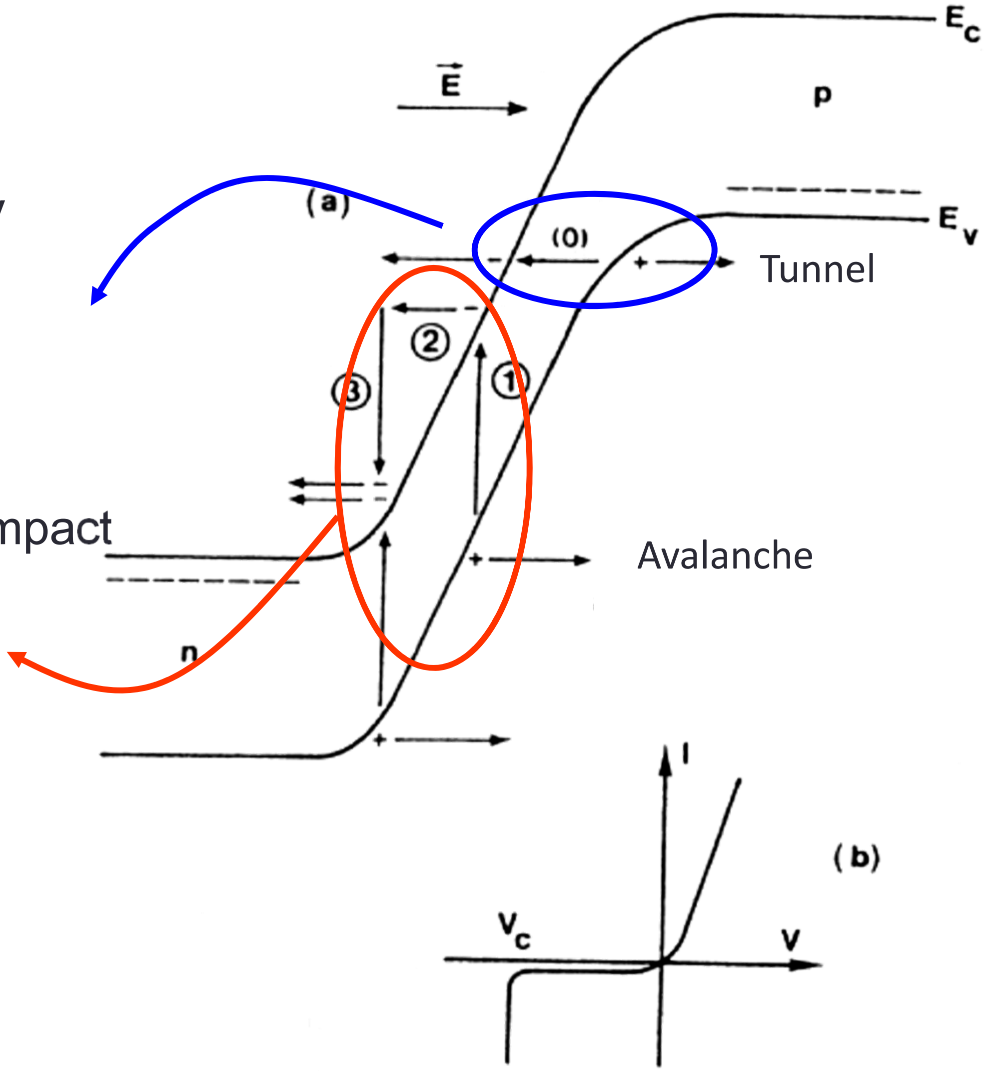
$$J(V) = J_0\left(\exp(\frac{eV_a}{nkT}) - 1\right)$$

Reverse biasing:
Junction breakdown

- Thermal Effect (Narrow bandgap)
- Zener Effect:
  - direct flowing from VB to CB by tunnel effect (0), if electric field above critical Field E_c
- Avalanche Effect:
  - before« tunneling », hot electrons (accelerated electrons) excite by impact ionisation electrons from VB to CB (1,2,3) etc….

$$V_{BD} = \frac{\varepsilon . E_C^2}{2eN_B}$$

- « Punchtrough »



Small signal model of the diode: capacitances

- Capacitance associated to charges
- 2 types of charges present in the junction
  - Fixed charges (ionised dopants) in depletion layer
  - Mobiles (e^- et h^+) injected when forward biasing
- 2 types of capacitance
  - Junction (or Transition) Capacitance
  - Charge Storage (or diffusion) Capacitance

Junction capacitance

Simply associated to charges present in depletion layer

$$C_T = C_j = \left|\frac{dQ}{dV}\right| \qquad |Q| = eAN_AW_P = eAN_DW_N$$

or:

$$C_T = C_j = \frac{A}{2}\sqrt{\frac{2e\varepsilon}{(V_D - V_A)}\frac{N_AN_D}{(N_A + N_D)}} = \frac{A\varepsilon}{W_T}$$

Charge Storage (diffusion) capacitance

- Reflects the delay between the voltage and current
- Associated with charges injected into the neutral regionsTraduit le retard entre la tension et le courant

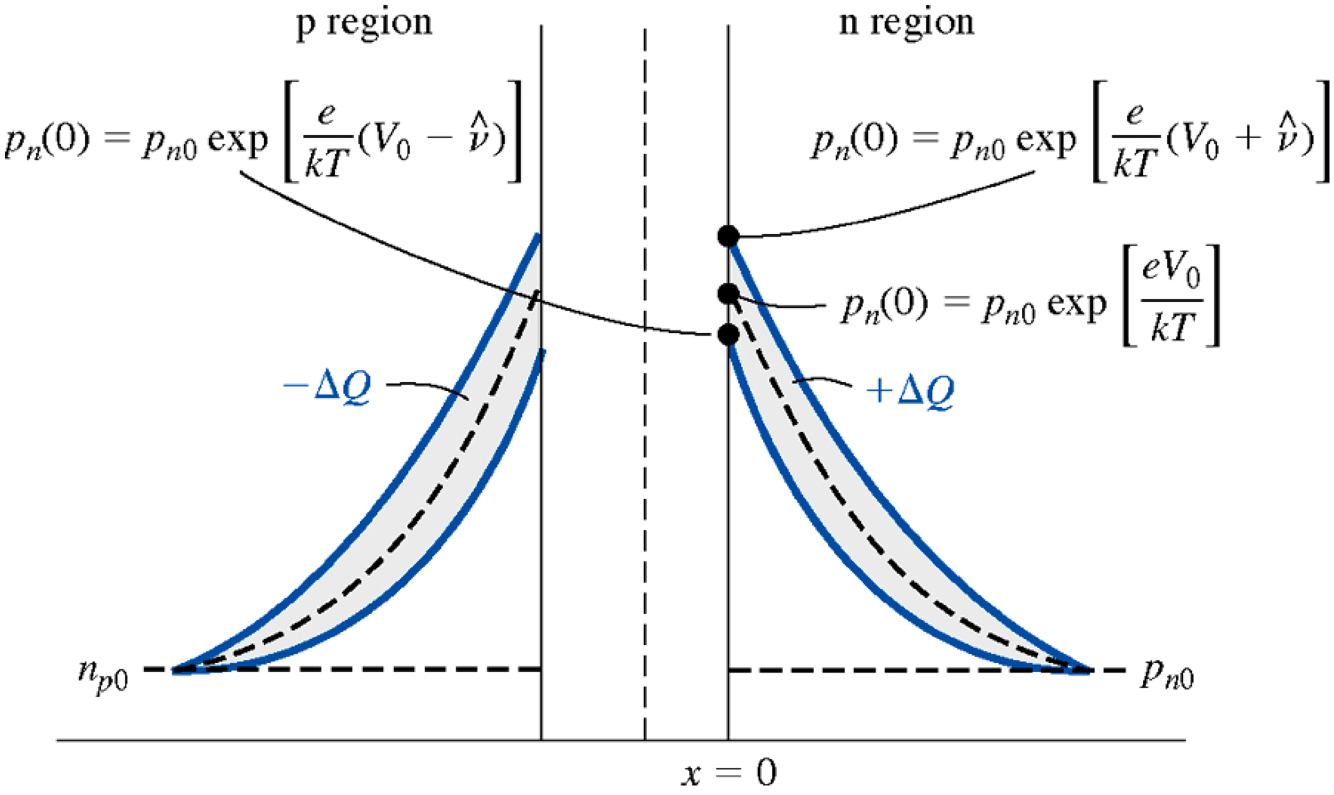
$$Q_{Sp} = A\int_{W_N}^{X_C} e(\underbrace{p'(x)-p_n}_{\text{Holes density in excess present in N region}})dx$$

$$Q_{Sp} = \tau_P J_P$$

$$Q_{Sn} = \tau_n J_n$$

$$Q_{Sp} = e(p'(0)-p_n)L_P\left[\coth(\frac{d_n}{L_P}) - \frac{1}{sh(\frac{d_n}{L_P})}\right]$$

Charge Storage (diffusion) capacitance



Charge Storage (diffusion) capacitance

- We can transform the previous expression by:

$$Q_{Sp} = \tau \; J_P(W_N) \qquad \text{avec} \qquad \tau = \tau_P \left(1 - \frac{1}{ch(\frac{d_n}{L_P})} \right)$$

- Time expression can be simplified, depending of the neutral geometry:
  - *Narrow diode*: $\tau_t = \frac{d_n^2}{2D_P}$ ⇔ transit time
  - *Long diode*: $\tau = \tau_P$ ⇔ lifetime

Charge Storage (diffusion) capacitance

- The previous expression, valid in N region, can be generalized in P region and we obtain for the whole diode:

$$Q_S = Q_{Sn} + Q_{Sp} = \tau_{(n)} J_n(-W_P) + \tau_{(p)} J_p(W_N)$$

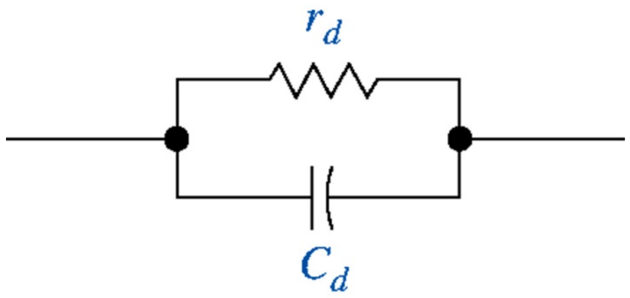
If we use:

$$C_S = C_d = \frac{dQ_S}{dV}$$

$$\boxed{C_S = C_d = C_{Sn} + C_{Sp} = \frac{e}{kT} K(\tau_{(n)} J_n + \tau_{(p)} J_p)}$$

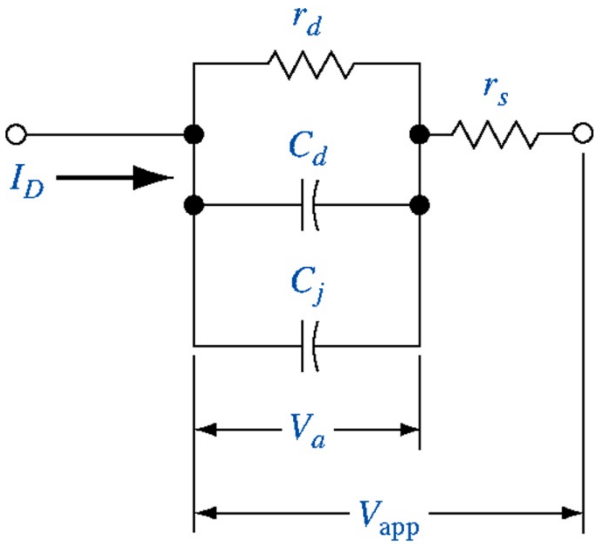
K : Geometry dependant Factor
(2/3 ⇔ narrow)
(1/2 ⇔ long)

Equivalent circuit of foward diode



(a)

(from Neamen)



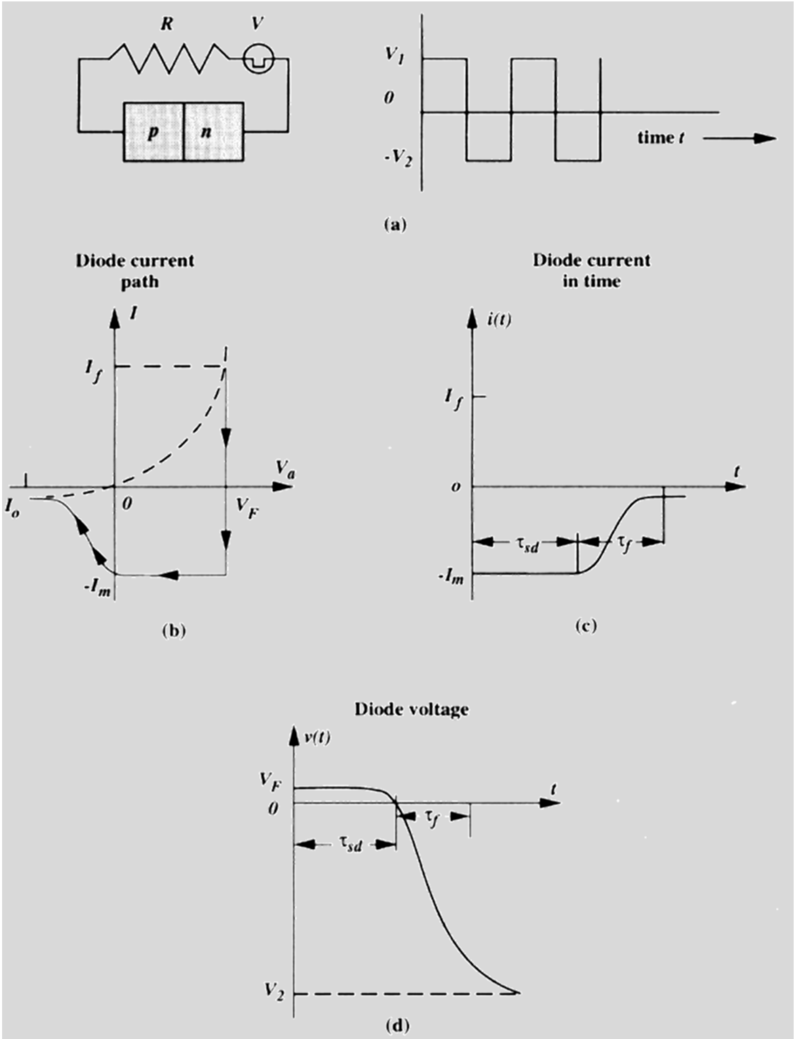
(b)

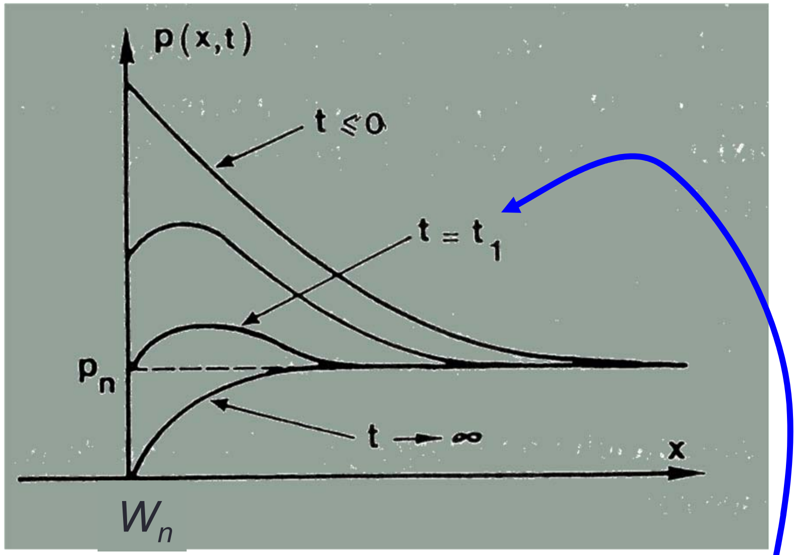
r_d : diode resistance (dynamic resistance) given by the differential slope of the I-V characteristics

$$r_d = \frac{kT}{e}\frac{1}{I}$$

r_s : serie resistance of neutral region n and p

Large signal switching of diode



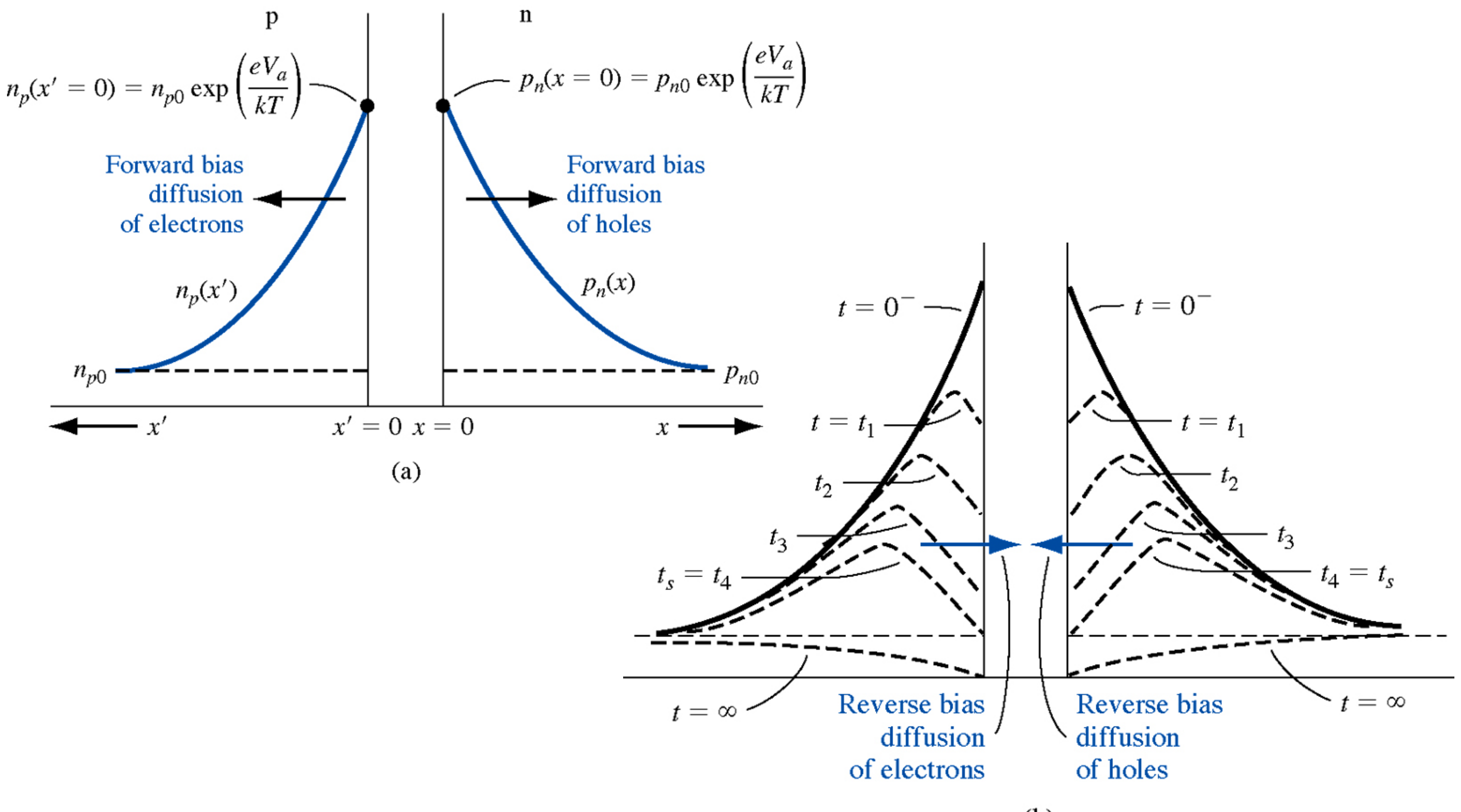


As long as the stored charge is positive ⇔ forward bias diode ⇔ voltage across diode is small (few 10 mV)

$$p'_n - p_n = p_n\left(e^{\frac{eV_a}{kT}} - 1\right)$$

τ_{sd} ⇔ Storage time *ie* $p'(W_N) = p_n$

Switching Junction PN



(a)

(b)

Large signal switching of diode

- Storage time :The main problem in minoritary carriers devices:
  - Storage time:

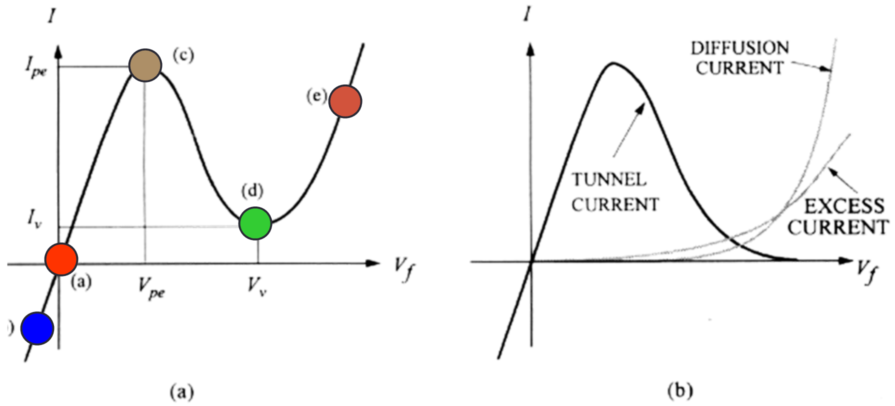
$$\boxed{\tau_{sd} \cong \tau_p \left[\ln(1+\frac{I_f}{I_m}) - \ln(1+\frac{I_f}{I_f+I_m}) \right]}$$

  - Rise (or fall) time :

$$\boxed{\tau_f \cong 2.3\left[\frac{\tau_F \delta + RC_j}{1+\delta}\right] \quad \text{avec } \delta = \frac{I_f}{I_f+I_m}}$$

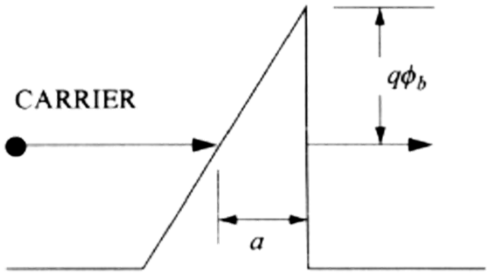
  - C_j: mean value of capacitance between zero and $-V_2$

Tunnel Diode –Backward diode

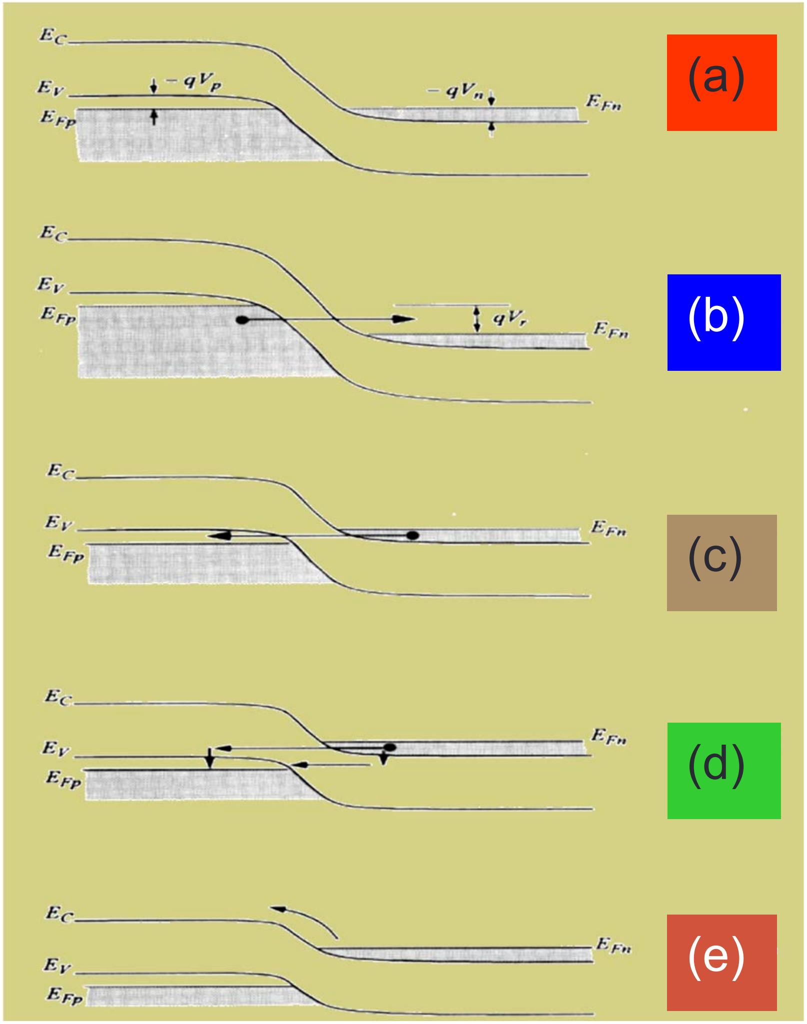


(a) (b)

$$I_t = I_{pe}\left(\frac{V_a}{V_{pe}}\right)\exp\left(1-\frac{V_a}{V_{pe}}\right)$$



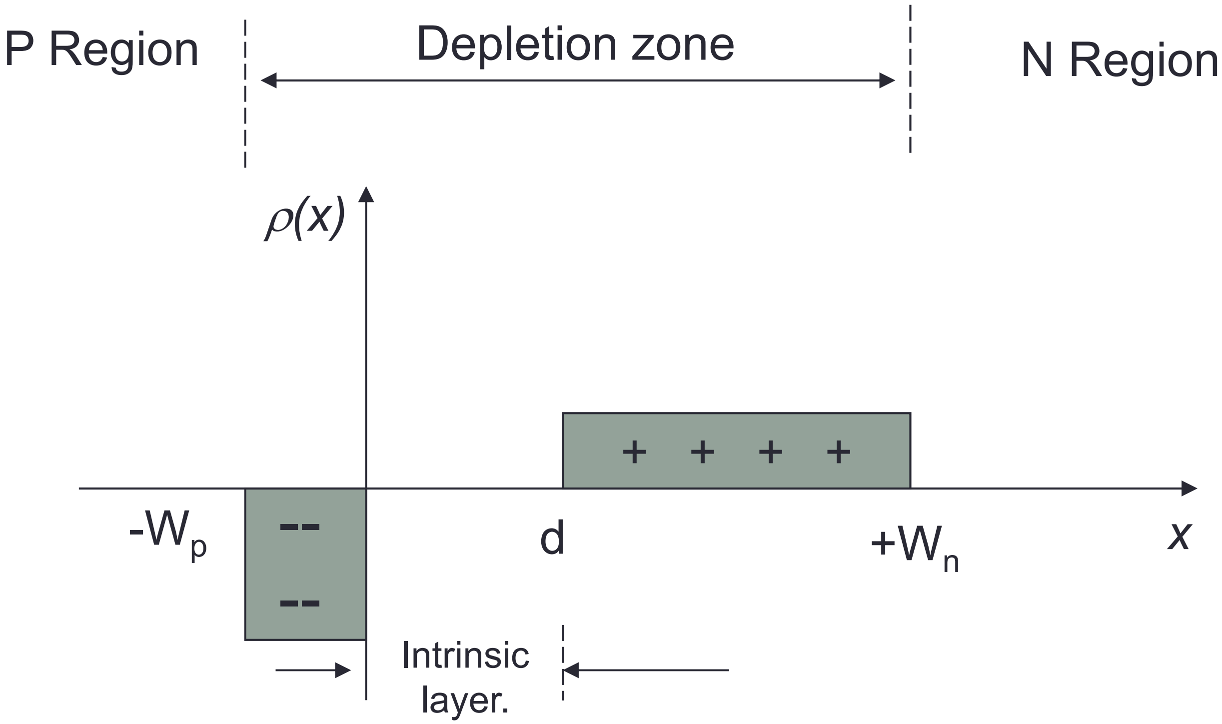
$$T_t \approx \exp\left(-\frac{4a\sqrt{2m^* e\phi_b}}{3\hbar}\right)$$



PIN Diodes

- VLSI devices ⇔ high electric fields
- Avalanche issues and hot electrons effects
- Solutions:
  - Reducing the electric field by increasing the space charge
  - Incorporation of an "undoped" layer called Intrinsic hence the name!

PIN Diodes


P Region
Depletion zone
N Region
$\rho(x)$
+ + + +
-- --
$-W_p$
d
$+W_n$
x
Intrinsic layer.

PIN Diodes

Max electric field (intrinsic zone)

$$E_m = -\frac{eN_A x_p}{\varepsilon_{Si}} = -\frac{eN_D(x_n - d)}{\varepsilon_{Si}}$$

built in potentiel

$$V_{bi} = \frac{|E_m|}{2}(x_p + x_n + d) = \frac{|E_m|}{2}(W_d + d)$$

space charge width

$$W_d = \sqrt{\frac{2\varepsilon_{Si}}{e}\frac{(N_A + N_D)}{N_A N_D}V_{bi} + d^2} = \sqrt{W_{d0}^2 + d^2}$$

capacity

$$\frac{C_T}{C_{T0}} = \frac{W_{d0}}{W_d} = \frac{1}{\sqrt{1 + \frac{d^2}{W_{d0}^2}}}$$

electric field

$$\frac{E_m}{E_{m0}} = \frac{W_d}{W_d + W_{d0}} = \sqrt{1 + \frac{d^2}{W_{d0}^2}} - \frac{d}{W_{d0}}$$