ECE 536 – Integrated Optics and Optoelectronics
Lecture 2 – January 20, 2022

Spring 2022

Tu-Th 11:00am-12:20pm

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Lecture 2 Outline

- More on EM for optics
- Concepts of Compound semiconductor materials introduced in Chapter 1
- Quick review of important concepts in Semiconductor electronics
- First HW assignment

Errata in Textbook

S.L. Chuang, "Physics of Photonic Devices," Wiley, 2nd Edition (2009)

A handout will be posted with the main errors which were found in the initial printings of the 2nd edition (may have been corrected in latest printings).

To these we should add:

- Equation 3.2.18 "=" should be ">"
  - $|z| > L/2$
- Equation 3.2.23 "=" should be "<"
  - $|z| < L/2$
- Equation 3.2.23: "L/2" not "L2" in exponent

Errata in Textbook

S.L. Chuang, "Physics of Photonic Devices," Wiley, 2nd Edition (2009)

Note these possible typos in Chapter 1 in formulas which are useful now:

1) Equation 1.3.1 should be:

$$a(A_xB_{1-x}C) = xa(AC) + (1-x)a(BC)$$

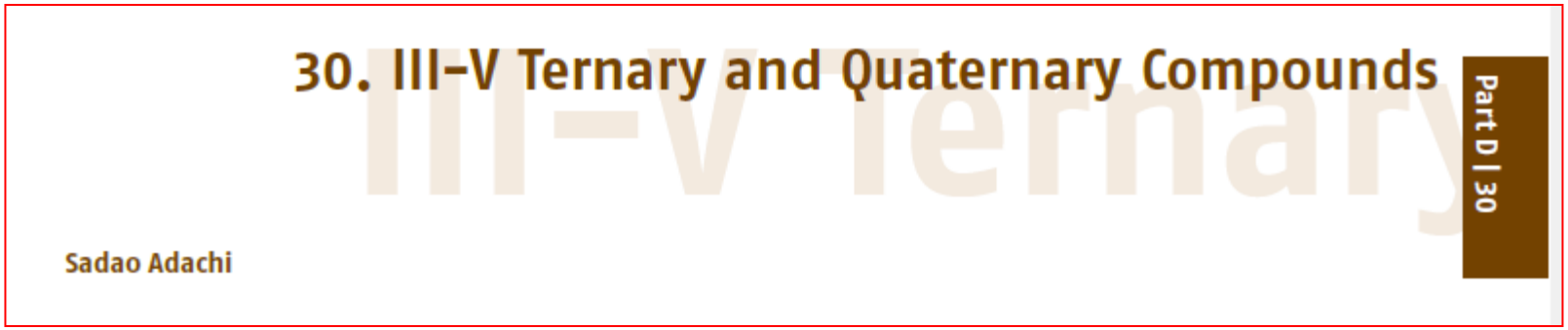
where a(AC) is the lattice constant of the binary compound AC and...

2) Equation 1.3.2 should be:

$$E_g(A_xB_{1-x}C) = xE_g(AC) + (1-x)E_g(BC) - bx(1-x)$$

Compound semiconductor materials

Chapter posted on the class website



S. Kasap, P. Capper (Eds.), *Springer Handbook of Electronic and Photonic Materials*, DOI 10.1007/978-3-319-48933-9_30

30.3 Structural Parameters

30.3.1 Lattice Parameters and Lattice-Matching Conditions Between III–V Quaternaries and Binary Substrates

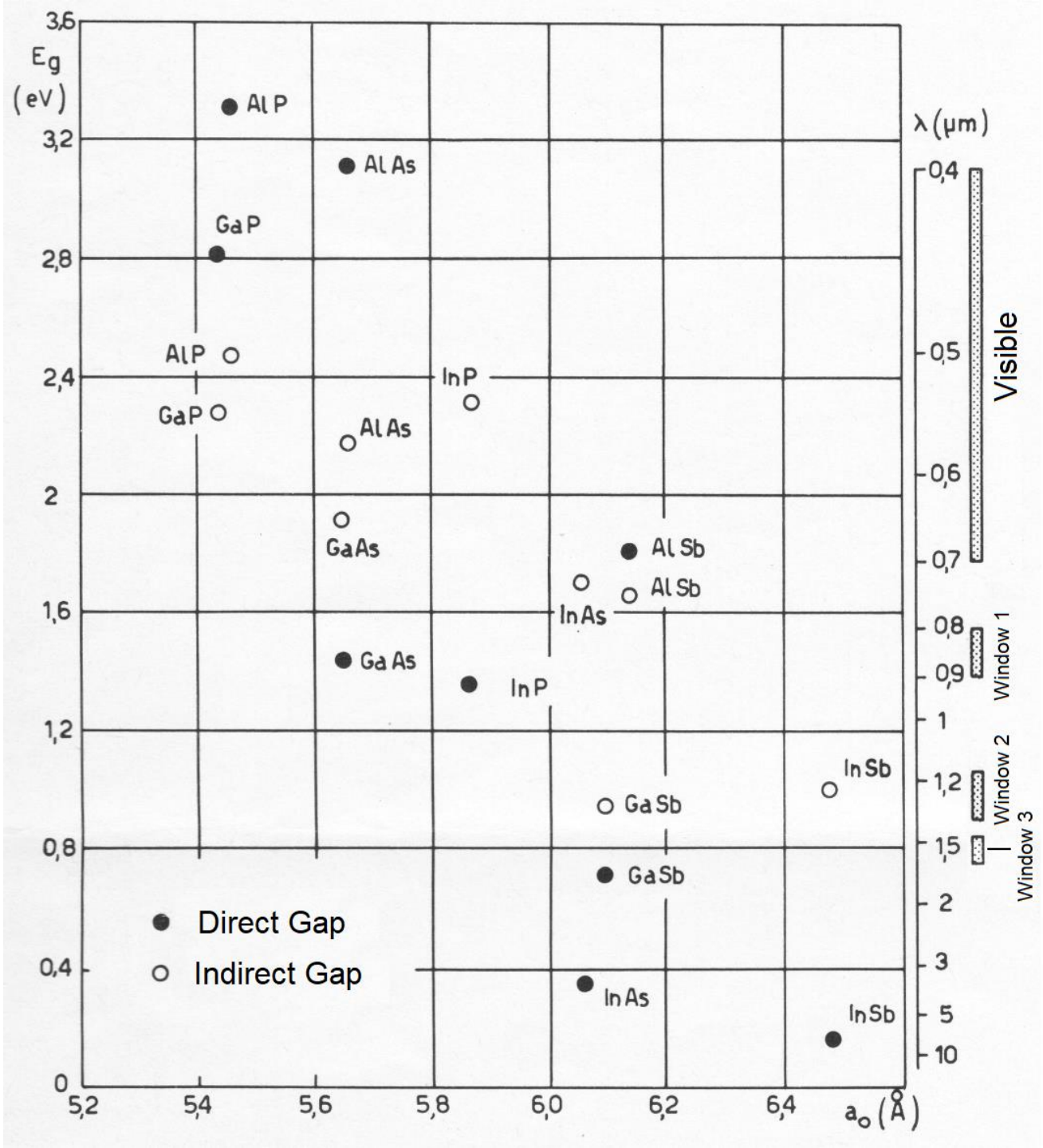
The lattice parameter a (c) is known to obey Vegard's law well, i. e., to vary linearly with composition. Thus, the lattice parameter for a III–V ternary can be simply obtained from (30.1) using the binary data listed in Table 30.1 [30.3, 4]. Introducing the lattice parameters in Table 30.1 into (30.3) [(30.5)], one can also obtain the lattice-matching conditions for $A_{1-x}B_xC_yD_{1-y}$ ($A_xB_yC_{1-x-y}D$) quaternaries on various III–V binary substrates (GaAs, GaSb, InP and InAs). These results are summarized in Tables 30.2, 30.3, 30.4 and 30.5.

$$T_{A_xB_{1-x}C} = xB_{AC} + (1-x)B_{BC} \equiv a + bx \qquad (30.1)$$

$$T_{A_xB_{1-x}C} = xB_{AC} + (1-x)B_{BC} + C_{A-B}x(1-x)$$
$$\equiv a + bx + cx^2 \,, \qquad (30.2)$$

bowing parameter

The playground of band gap engineering



Al P
Al As
Al Sb
Ga P
Ga As
Ga Sb
In P
In As
In Sb

Without considering
boron (B)
nitrogen (N)
thallium (Tl)
bismuth (Bi)

9 binary compounds

18 ternary alloys

$A_x B_{1-x} C$ 2:1

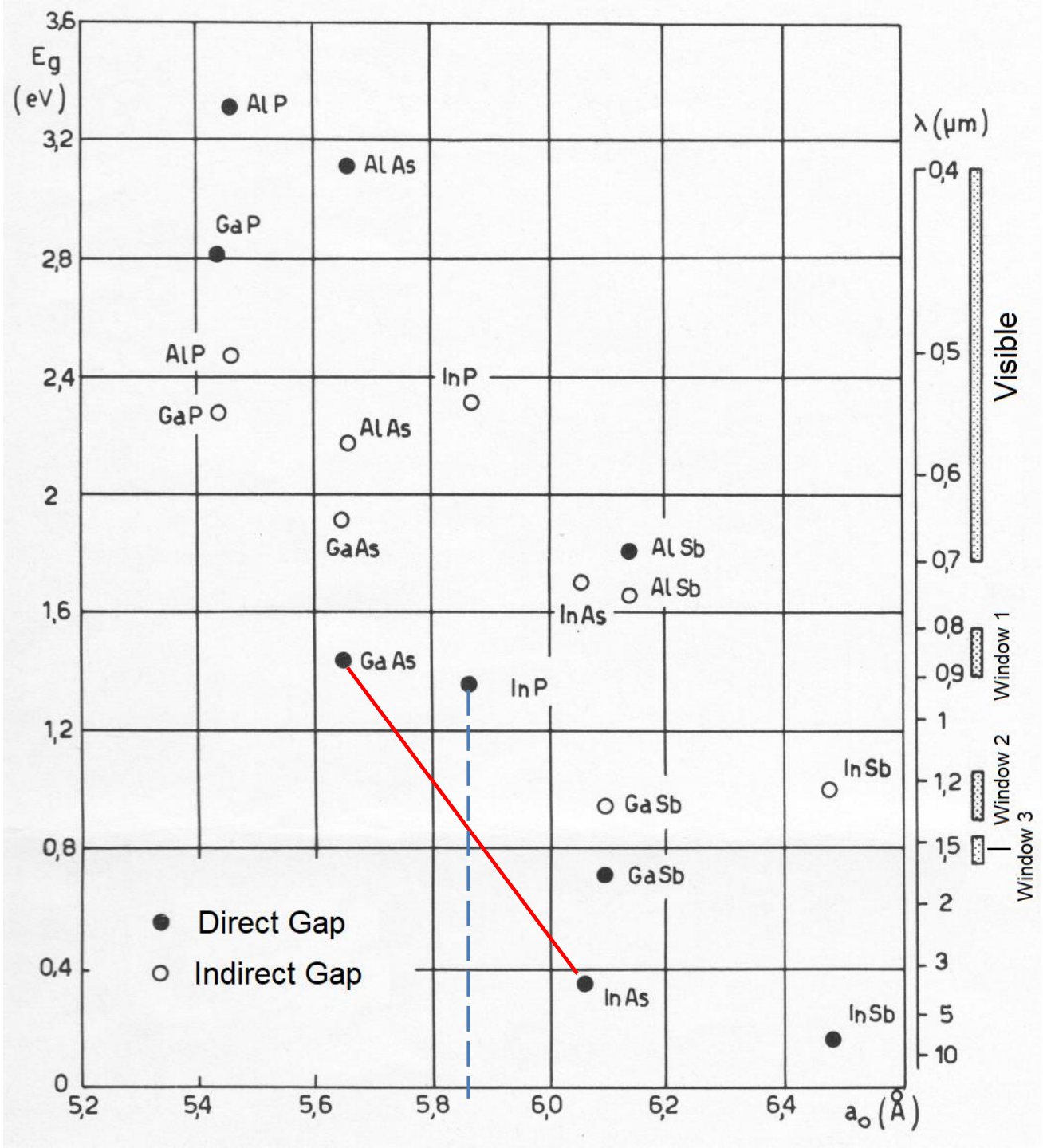
$A C_y D_{1-y}$ 1:2

quaternary alloys

$A_x B_{1-x} C_y D_{1-y}$ 2:2

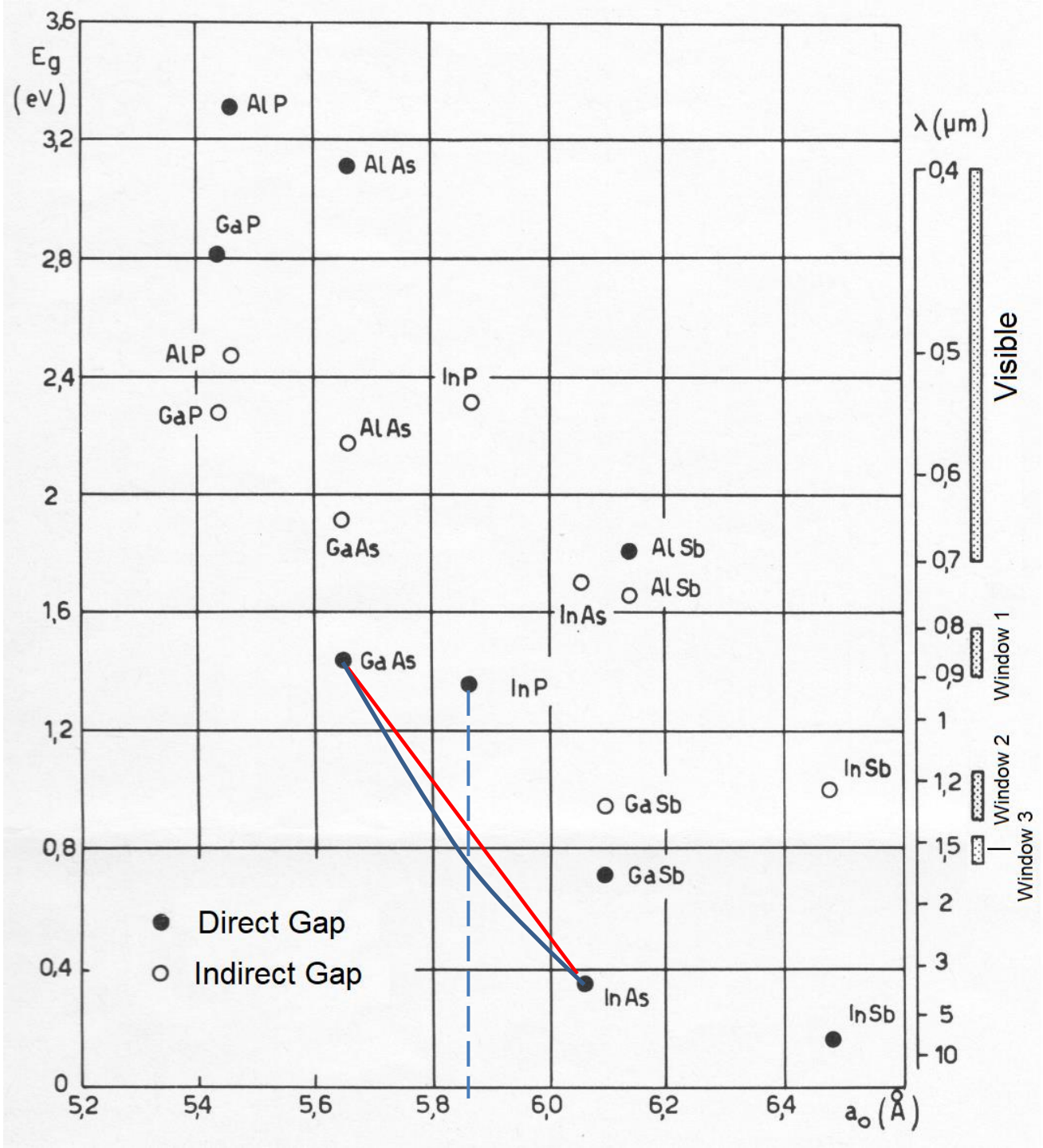
$A_x B_y C_{1-x-y} D$

1:3 or 3:1



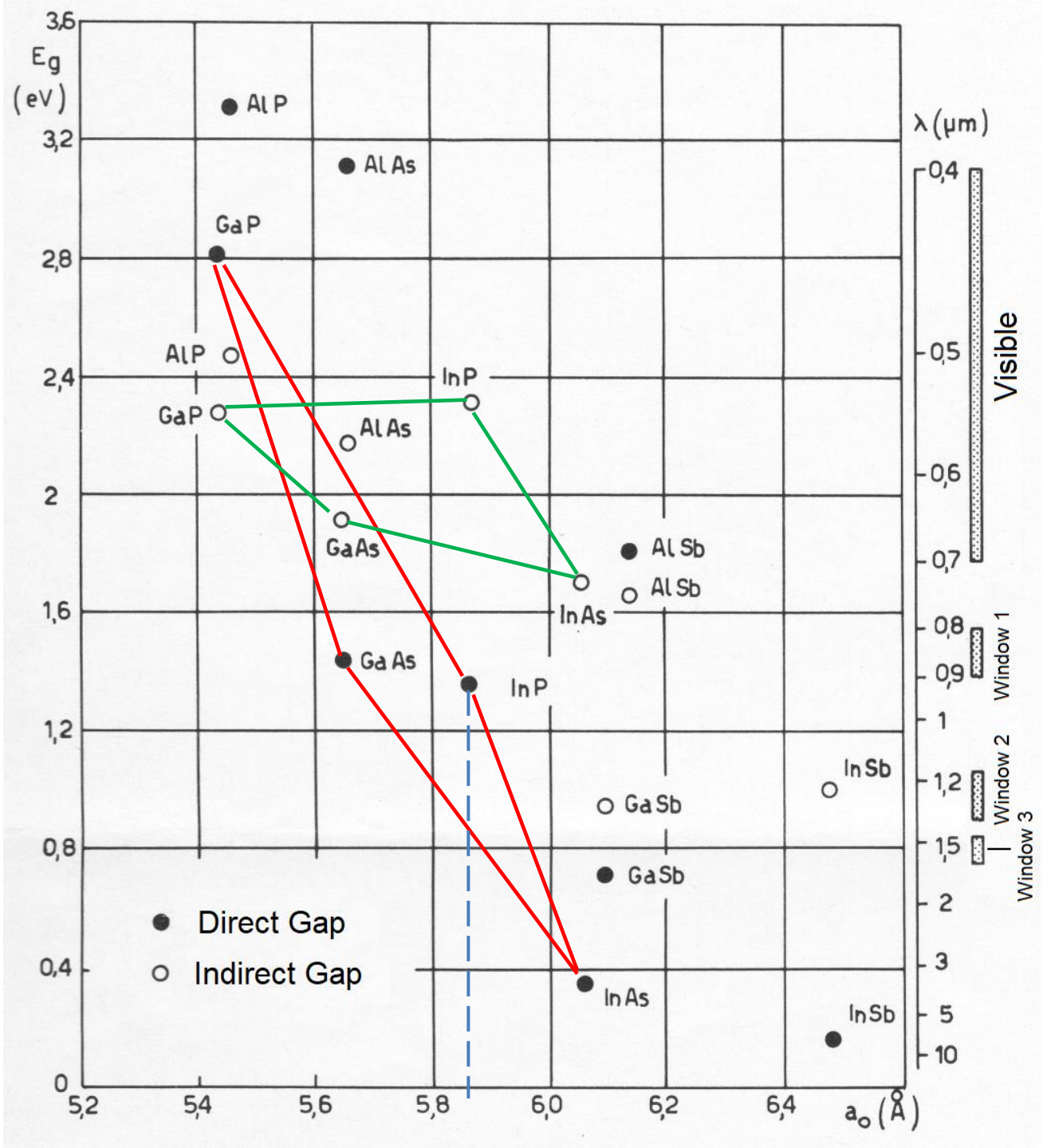
Linear approximation

$In_x Ga_{1-x} As$ 2:1

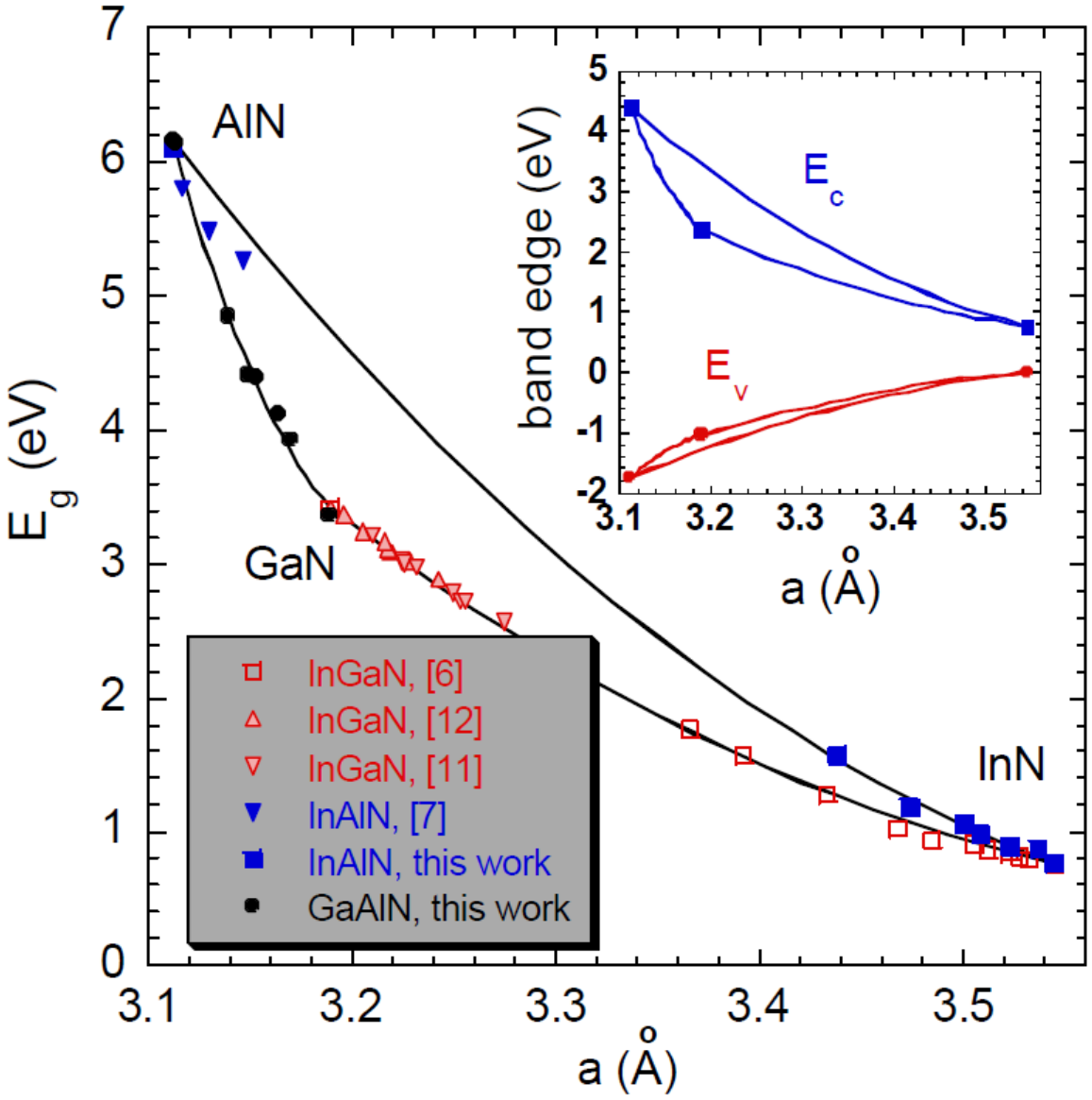


Including bowing

$In_x Ga_{1-x} As$ 2:1



$Ga_x In_{1-x} As_y P_{1-y}$ 2:2



Example for Nitride materials

Solid State Communications 127 (2003) 411–414

Universal bandgap bowing in group-III nitride alloys

J. Wu[a,b,*], W. Walukiewicz[b], K.M. Yu[b], J.W. Ager III[b], S.X. Li[b,c], E.E. Haller[b,c], Hai Lu[d], William J. Schaff[d]

Semiconductor Electronics
Quick Review

In most application of optoelectronic semiconductor devices the attention is not on high-field hot-carrier transport, as is the case for microwave devices and highly scaled MOSFETs.

Although devices generate or interact with extremely high frequency EM waves, the transport of electrons and holes is well described by the standard semiconductor equations based on drift-diffusion.

The interaction between photons and mobile charges is mostly based on quantum mechanics concepts.

Poisson's Equation

$$\nabla \bullet (\varepsilon \nabla \phi) = -\rho$$

- Relates charge density to the scalar potential
- ε can be a scalar or a tensor depending upon material properties

Where:

$$\rho = q\left(p - n + N_D^+ - N_A^-\right) = q\left(p - n + C_0\right)$$

$C_0 \equiv N_D^+ - N_A^-$ and $q = 1.6 \times 10^{-19}\,\mathrm{C}$ (unit charge)

Note: If $\rho = 0$, this becomes the charge neutrality equation: $n - p = N_D^+ - N_A^-$

Carrier Transport Equations

Drift-diffusion equations

Express the behavior of Boltzmann equation close to equilibrium conditions

$$\mathbf{J_n} = q\mu_n n\mathbf{E} + qD_n \nabla n$$
$$\mathbf{J_p} = q\mu_p p\mathbf{E} - qD_p \nabla p$$

Einstein Relation: $\frac{D}{\mu} = \frac{kT}{q}$ so

$$\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{kT}{q}$$

$\mathbf{E} = -\nabla\phi$

μ_n is the electron mobility (not permeability μ)

μ_p is the hole mobility

D_n is the electron diffusion coefficient

D_p is the hole diffusion coefficient

Continuity Equations

These are charge conservation laws, which in differential form are related to the behavior of the divergence of charge flow. They descend formally from Maxwell's equations.

Starting with Ampere's Law: $\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial}{\partial t}\mathbf{D}$

$\mathbf{J}$ is composed of electron and hole currents: $\mathbf{J} = \mathbf{J}_{\mathbf{con}} = \mathbf{J}_{\mathbf{n}} + \mathbf{J}_{\mathbf{p}}$

Using the vector identity $\nabla \bullet \left(\nabla \times \mathbf{A}\right) = 0$ (the divergence of the curl is zero):

$$0 = \nabla \bullet \left(\nabla \times \mathbf{H}\right) = \nabla \bullet \left(\mathbf{J} + \frac{\partial}{\partial t}\mathbf{D} \right) = \nabla \bullet \mathbf{J} + \nabla \bullet \left(\frac{\partial}{\partial t}\mathbf{D} \right) = \nabla \bullet \mathbf{J} + \frac{\partial}{\partial t}\nabla \bullet \mathbf{D} = \nabla \bullet \mathbf{J}_{\mathbf{con}} + \frac{\partial}{\partial t}\nabla \bullet \mathbf{D}$$

since $\nabla \bullet \mathbf{D} = \rho$ (Gauss's Law): $\nabla \bullet \mathbf{J}_{\mathbf{con}} + \frac{\partial}{\partial t}\rho = 0$

Continuity Equations

Using the expression $\rho = q\left(p - n + N_D^+ - N_A^-\right) = q\left(p - n + C_0\right)$ and realizing $\frac{\partial C_0}{\partial t} = 0$:

$$\nabla \bullet \left(\mathbf{J_n} + \mathbf{J_p}\right) + q\frac{\partial}{\partial t}\left(p - n\right) = 0 \quad \text{or} \quad \left(\nabla \bullet \mathbf{J_n} - q\frac{\partial}{\partial t}n\right) + \left(\nabla \bullet \mathbf{J_p} + q\frac{\partial}{\partial t}p\right) = 0$$

$$\text{so} \quad \left(\nabla \bullet \mathbf{J_n} - q\frac{\partial}{\partial t}n\right) = -\left(\nabla \bullet \mathbf{J_p} + q\frac{\partial}{\partial t}p\right) \equiv qR$$

R is the net recombination rate of electron-hole pairs with units of $\text{cm}^{-3}\text{s}^{-1}$

In cases where there is both generation and recombination:

$R = R_n - G_n$ (electrons) and $R = R_p - G_p$ (holes) and so

$$\frac{\partial n}{\partial t} = G_n - R_n + \frac{1}{q}\nabla \bullet \mathbf{J_n} \quad \text{and} \quad \frac{\partial p}{\partial t} = G_p - R_p - \frac{1}{q}\nabla \bullet \mathbf{J}_p \quad \Leftarrow \text{ Continuity Equations}$$

The classical "Semiconductor Equations"

- Using the carrier transport equations and the continuity equations:

$$\frac{\partial n}{\partial t} = G_n - R_n + \frac{1}{q}\nabla \bullet \mathbf{J_n} = G_n - R_n + \frac{1}{q}\nabla \bullet \left[q\mu_n n\mathbf{E} + qD_n \nabla n\right]$$

$$= G_n - R_n + \frac{1}{q}\nabla \bullet \left[-q\mu_n n\nabla\phi + qD_n \nabla n\right]$$

$$\frac{\partial p}{\partial t} = G_p - R_p - \frac{1}{q}\nabla \bullet \mathbf{J_p} = G_p - R_p - \frac{1}{q}\nabla \bullet \left[q\mu_p n\mathbf{E} - qD_p \nabla p\right]$$

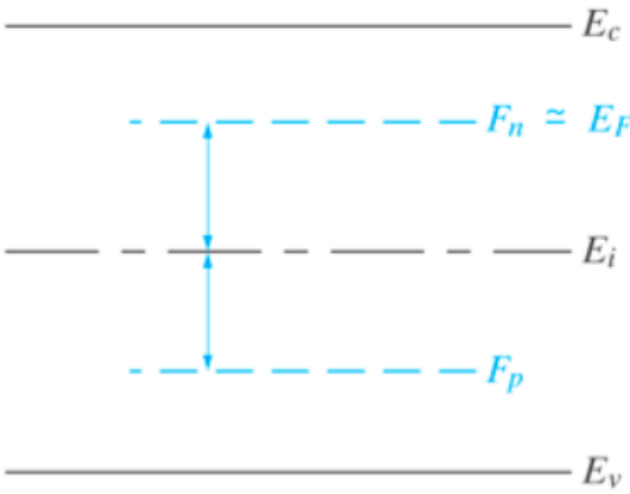
$$= G_p - R_p - \frac{1}{q}\nabla \bullet \left[-q\mu_p p\nabla\phi - qD_p \nabla p\right]$$

- Considering also Poisson's Equation

$$\nabla \bullet (\varepsilon \nabla \phi) = -q(p - n + C_0)$$

- These give 3 equations in 3 unknowns, which with the boundary conditions can be used to solve for n, p, and ϕ

Alternative description: Quasi-Fermi levels



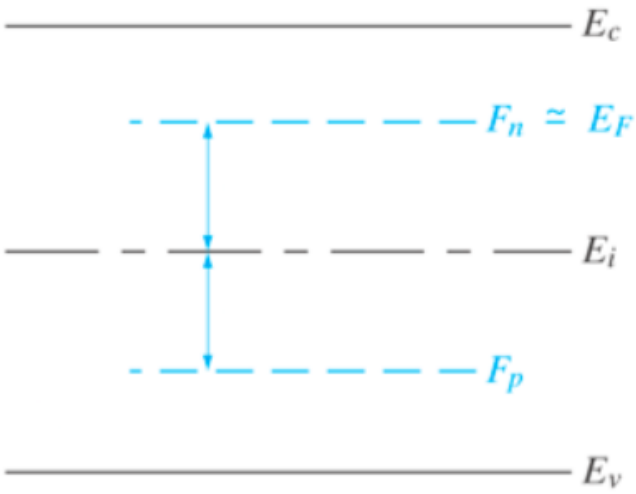
For a non-degenerate semiconductor:

$$n(x,y,z) = n_i e^{\left[\frac{F_n(x,y,z) - E_i(x,y,z)}{k_B T}\right]}$$

$$p(x,y,z) = n_i e^{\left[\frac{E_i(x,y,z) - F_p(x,y,z)}{k_B T}\right]}$$

F_n and F_p are the quasi-Fermi levels

Alternative description: Quasi-Fermi levels



Intrinsic Carrier Concentration: $n_i = \sqrt{N_C N_V}\, e^{-E_g/(2k_BT)}$

Intrinsic Energy Level: $E_i(x,y,z) = -q\phi(x,y,z) + E_{ref}$

Where E_{ref} is the system constant energy reference

Quasi-Fermi Energies:

$$F_n(x,y,z) = -q\phi_n(x,y,z) + E_{ref}$$

$$F_p(x,y,z) = -q\phi_p(x,y,z) + E_{ref}$$

Carrier Distributions: General Case

$$n = \int_{-\infty}^{\infty} f_n(E)\rho_e(E)dE$$

$$p = \int_{-\infty}^{\infty} f_p(E)\rho_h(E)dE$$

where $\rho_e(E)$ and $\rho_h(E)$ are the electron and hole density of states (respectively) and $f(E)$ is the Fermi-Dirac Distribution

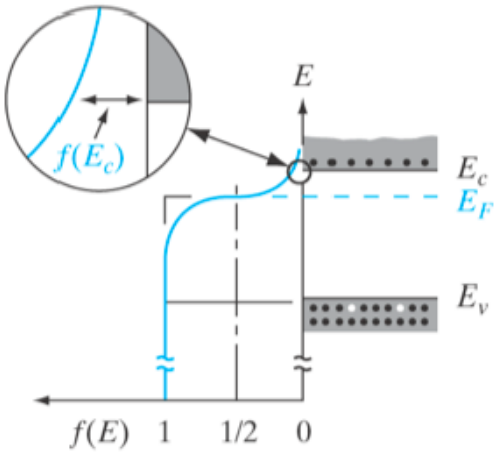
$$f(E) = \frac{1}{1+e^{(E-E_F)/k_BT}}$$

For Electrons: $f_n(E) = \frac{1}{1+e^{(E-F_n)/k_BT}}$

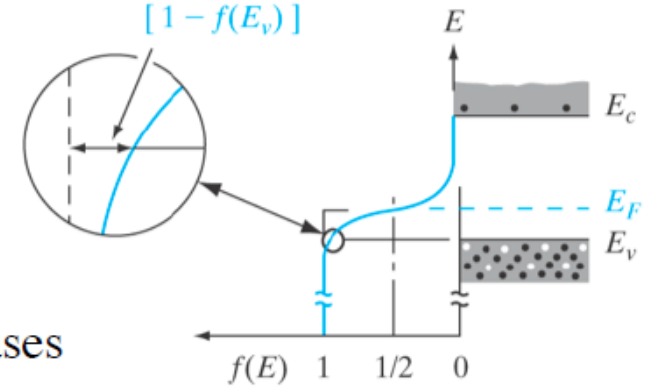
For Holes: $f_p(E) = 1 - f(E) = \frac{1}{1+e^{(F_p-E)/k_BT}}$

$\Rightarrow$ Applies to both degenerate and non-degenerate cases

Fermi Distribution (n-type)

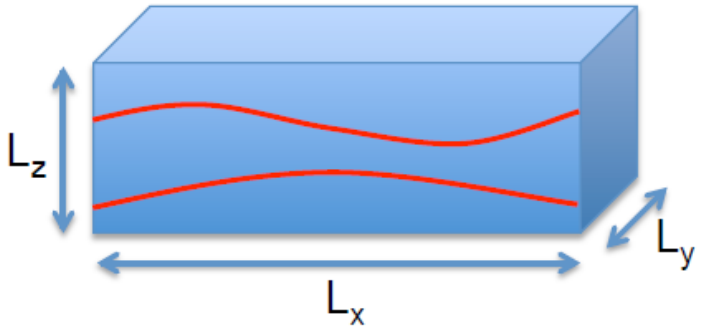


Fermi Distribution (p-type)



Density of states

In a volume of finite size defined by lengths L_x, L_y, and L_z, the electron can be approximated as a "free electron" with discrete values for the wave number which must satisfy the relations:



$$k_x = m\frac{\pi}{L_x}, \quad k_y = n\frac{\pi}{L_y}, \quad k_z = l\frac{\pi}{L_z}$$

where m, n, and l are positive integers.

The energy of an electron with wave numbers k_x, k_y, k_z is:

$$E = \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2 + k_z^2\right)$$

Each set of k vectors represents a state, and 2 electrons can occupy a single state. The number of electrons per unit volume is found by summing the probability of individual state occupancy over the total number of states:

$$n = \frac{2}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} f_n(E)$$

Density of states

The set of allowed energies (states) can be thought of as a lattice of discrete points in k-space defined by unit vectors of length $\left(\frac{\pi}{L_x}\right)$, $\left(\frac{\pi}{L_y}\right)$, and $\left(\frac{\pi}{L_z}\right)$

The number of lattice points contained in a k-space region with size $dk_x \times dk_y \times dk_z$ is therefore: $\frac{dk_x dk_y dk_z}{\pi^3} V$

As the volume increases, the spacing between allowed energies decreases and the sum of the previous slide can be replaced by an integral:

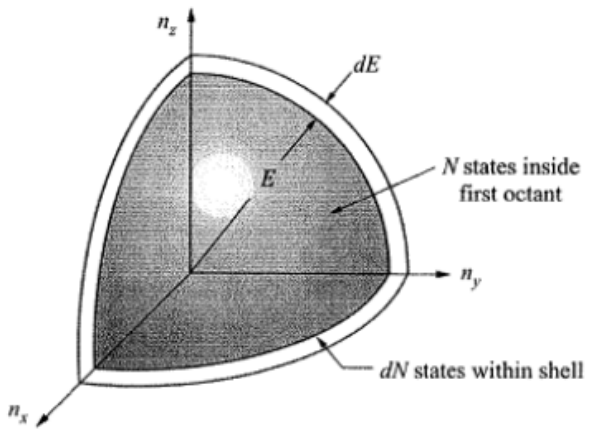
$$n = \frac{2}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} f_n(E) = \frac{2}{\pi^3}\int_0^\infty\int_0^\infty\int_0^\infty dk_x\, dk_y\, dk_z f_n(E)$$

Density of states

Consider a system using the parabolic band model with spherical symmetry:

The number of states below an energy E is formed by an eighth sphere in k-space:

$$N(E) = \frac{2}{\pi^3}\int_V d^3k = \frac{2}{\pi^3}\left(\frac{1}{8}\cdot\frac{4}{3}\pi k^3\right) = \frac{1}{3\pi^2}k^3$$



$$\text{Using } E = E_C + \frac{\hbar^2 k^2}{2m_e^*} \Rightarrow k = \left(\frac{2m_e^*}{\hbar^2}\right)^{1/2}\left(E - E_C\right)^{1/2}$$

$$N(E) = \frac{1}{3\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\left(E - E_C\right)^{3/2}$$

$$\rho_e(E) = \frac{dN(E)}{dE} = \frac{3}{2}\cdot\frac{1}{3\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\left(E - E_C\right)^{1/2} = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\left(E - E_C\right)^{1/2} \text{ for } E > E_C$$

Similarly for holes:

$$\rho_h(E) = \frac{dN(E)}{dE} = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}\left(E_V - E\right)^{1/2} \text{ for } E < E_V$$

Density of states

From the previous slides:

$$n = \int_{-\infty}^{\infty} f_n(E)\rho_e(E)dE = \int_{-\infty}^{\infty} \frac{1}{1+e^{(E-F_n)/k_BT}} \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\left(F_n - E_C\right)^{1/2} dE$$

$$p = \int_{-\infty}^{\infty} f_p(E)\rho_h(E)dE = \int_{-\infty}^{\infty} \frac{1}{1+e^{(F_p-E)/k_BT}} \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}\left(E_V - F_p\right)^{1/2} dE$$

Using the Fermi-Dirac integral:

$$F_j(\eta) = \frac{1}{\Gamma(j+1)}\int_0^{\infty} \frac{x^j dx}{1+e^{(x-\eta)}}$$

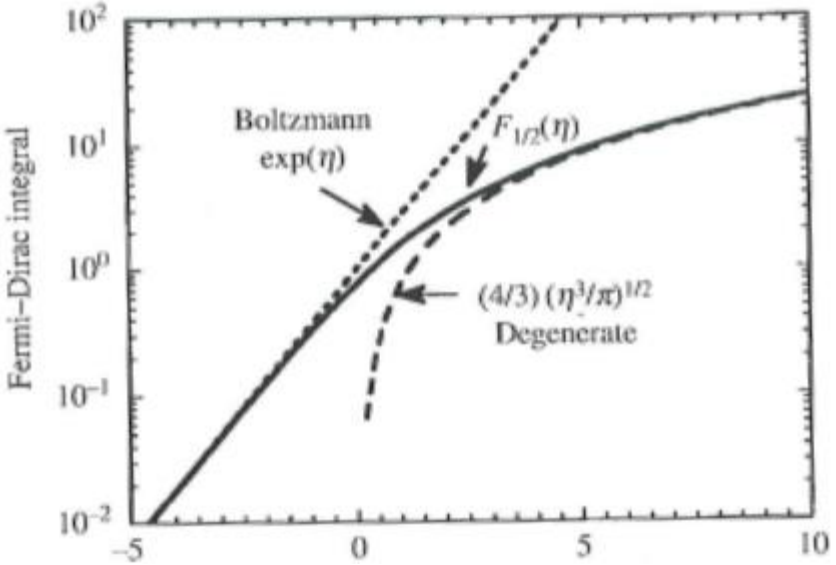
$$n = N_C F_{1/2}\left(\frac{F_n - E_C}{k_BT}\right) \quad \text{where} \quad N_C = 2\left(\frac{m_e^* k_BT}{2\pi\hbar^2}\right)^{3/2} = 2.51\times10^{19}\left(\frac{m_e^*}{m_o}\frac{T}{300}\right)^{3/2} cm^{-3}$$

$$p = N_V F_{1/2}\left(\frac{E_V - F_p}{k_BT}\right) \quad \text{where} \quad N_V = 2\left(\frac{m_h^* k_BT}{2\pi\hbar^2}\right)^{3/2} = 2.51\times10^{19}\left(\frac{m_h^*}{m_o}\frac{T}{300}\right)^{3/2} cm^{-3}$$

Approximation of Fermi-Dirac Integral

The Fermi-Dirac integral is defined as:

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j dx}{1 + e^{(x-\eta)}}$$



An approximate analytical form is given by:

$$F_j(\eta) = \frac{1}{e^{-\eta} + C_j(\eta)}$$

For j = $\frac{1}{2}$, the expression for C giving an error of less than 0.5% is:

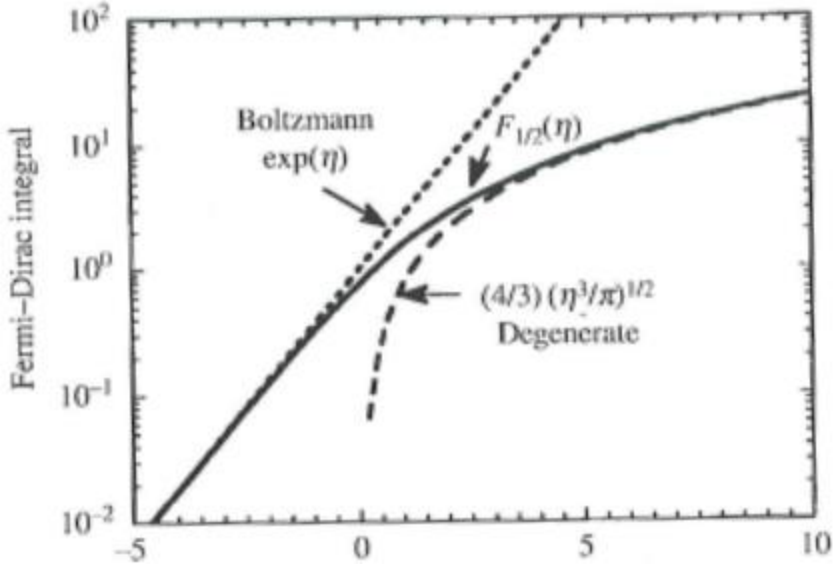
$$C_{1/2}(\eta) = \frac{3(\pi/2)^{1/2}}{\left[\eta + 2.13 + \left(|\eta - 2.13|^{12/5} + 9.6\right)^{5/12}\right]^{3/2}}$$

Approximation of Fermi-Dirac Integral

Another approximation of the Fermi-Dirac integral valid for $|\eta| \gg 1$ and j = 1/2 is:

$$F_{1/2}(\eta) \sim e^{\eta} \qquad \text{for } \eta \ll -1$$

$$\sim \frac{4}{3}\left(\frac{\eta^3}{\pi}\right)^{1/2} \qquad \text{for } \eta \gg 1$$



Approximate Inverse (Nilsson, 1973)

$$\eta = \frac{\ln(u)}{1-u} + v - \frac{v}{1+(0.24+1.08v)^2}$$

$$u = F_{1/2}(\eta) \qquad v = \left(3\sqrt{\pi}\cdot u/4\right)^{2/3}$$

Determination of Fermi level

Consider a bulk semiconductor in equilibrium

Charge Neutrality: $n_o + N_A^- = p_o + N_D^+$

N_A^- is the ionized acceptor concentration and N_D^+ is the ionized donor concentration

In the simplified model, $N_D^+ \sim N_D$ but more specifically:

$$N_A^- = (\text{Density of Acceptors}) \times (\text{Probability State is Filled})$$

$$= N_A \times \frac{1}{1 + g_A e^{(E_A - E_F)/k_B T}} = \frac{N_A}{1 + g_A e^{(E_A - E_F)/k_B T}}$$

g_A is the ground state degeracy factor for acceptors

Determination of Fermi level

For common semiconductors $g_A = 4:$ 2 spin states, 2 degenerate bands (lh, hh)

Similarly for donors:

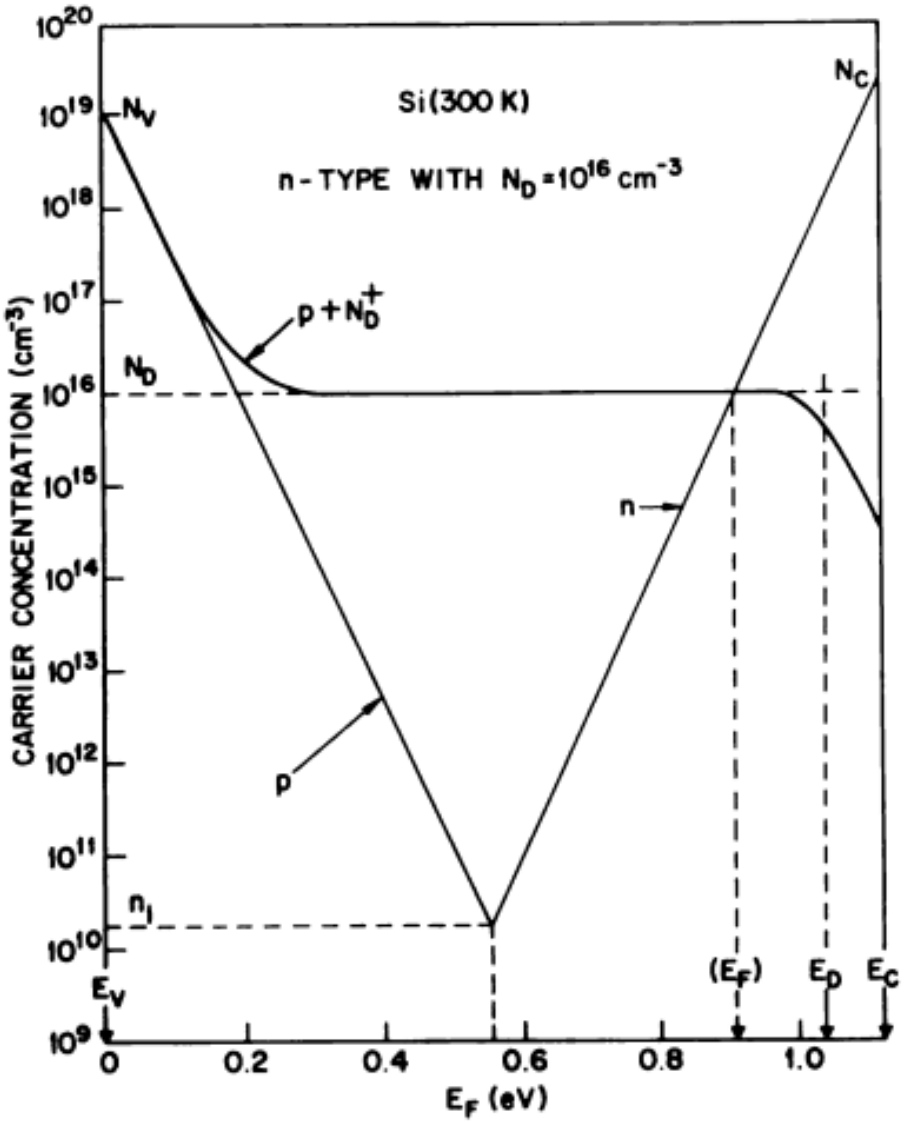
$$N_D^+ = (\text{Density of Donors}) \times (\text{Probability State is Empty})$$

$$= N_D \left[1 - \frac{1}{1 + \frac{1}{g_D} e^{(E_D - E_F)/k_B T}} \right] \Longrightarrow = N_D \frac{1}{1 + g_D \exp\left(\frac{E_F - E_D}{k_B T} \right)}$$

g_D is the donor ground state degeneracy, and $g_D = 2$ (2 spin states)

Using the expressions for N_A^- and N_D^+ with charge neutrality the Fermi Energy can be determined.

Determination of Fermi level



$$n = N_D^+ + p$$

n

$$N_C \exp\left(-\frac{E_C - E_F}{kT}\right) =$$

N_D^+

$$= N_D \frac{1}{1 + 2\exp\left(\frac{E_F - E_D}{kT}\right)} +$$

p

$$+ N_V \exp\left(\frac{E_V - E_F}{kT}\right)$$

W. Shockley, *Electrons and Holes in Semiconductors*, D. Van Nostrand, Princeton, N.J., 1950.

Determination of Fermi level

Assuming a nondegenerate case:

$$n_o = n_i e^{(E_F - E_i)/k_B T} = N_C e^{(E_F - E_C)/k_B T}$$

$$p_o = n_i e^{(E_i - E_F)/k_B T} = N_V e^{(E_V - E_F)/k_B T}$$

In equilibrium, by multiplying these expressions it can be seen:

$$n_o p_o = n_i e^{(E_F - E_i)/k_B T} n_i e^{(E_i - E_F)/k_B T} = n_i^2$$

$$= N_C e^{(E_F - E_C)/k_B T} N_V e^{(E_V - E_F)/k_B T} = N_C N_V e^{-E_g/k_B T}$$

For n-type material, $N_D^+ - N_A^- \gg n_i$

$$n_o \simeq N_D^+ - N_A^- \text{ and } p_o = n_i^2 / \left(N_D^+ - N_A^-\right)$$

For p-type material, $N_A^- - N_D^+ \gg n_i$

$$p_o \simeq N_A^- - N_D^+ \text{ and } n_o = n_i^2 / \left(N_A^- - N_D^+\right)$$

The expression for the intrinsic energy can be shown to be:

$$E_i = \frac{E_C + E_V}{2} + \frac{3k_B T}{4} \ln\left(\frac{m_h^*}{m_e^*}\right)$$

Light Hole Effects

Total hole concentration: $p = p_{hh} + p_{lh}$

$$p_{hh} = N_V^{hh} F_{1/2}\left(\frac{E_v - E_F}{k_B T}\right) \quad \text{where} \quad N_V^{hh} = 2\left(\frac{m_{hh}^* k_B T}{2\pi\hbar^2}\right)$$

and

$$p_{lh} = N_V^{lh} F_{1/2}\left(\frac{E_v - E_F}{k_B T}\right) \quad \text{where} \quad N_V^{lh} = 2\left(\frac{m_{lh}^* k_B T}{2\pi\hbar^2}\right)$$

ASSIGNMENTS:

Reading Assignments
Chuang – Chapter 1, Section 2.2

Coldren & Corzine – Chapter 1 (Supplemental)

Paper by Adachi (2017) posted on class website

For a concise refresher of semiconductors you could also consider:
Chapter 1 of the classic book "Physics of Semiconductor Devices" 3rd edition (2007) by S.M. Sze and K.K. Ng, which you can freely download from our library.

Also available at:
https://archive.org/details/PhysicsOfSemiconductorDevices_855/page/n221/mode/2up