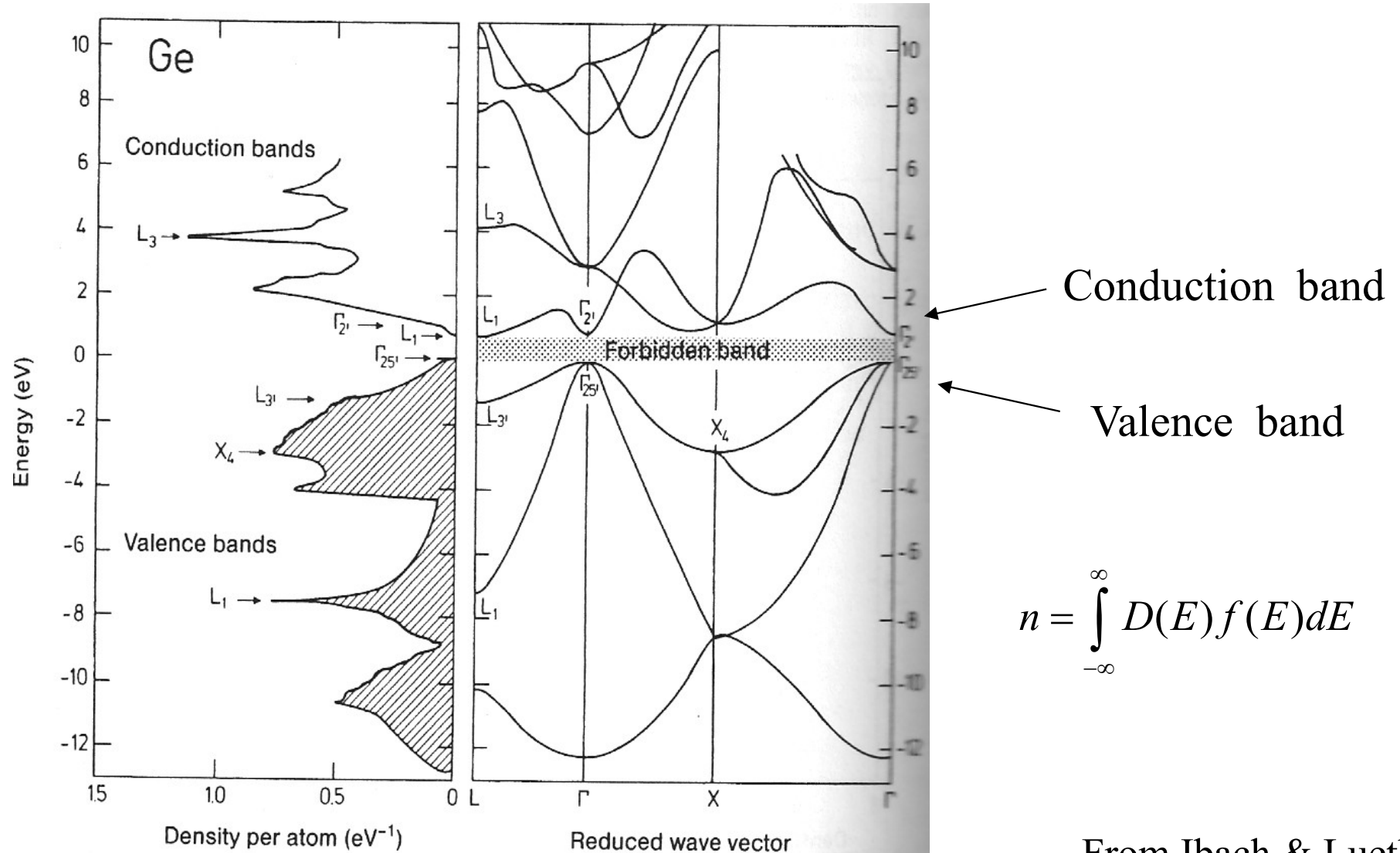


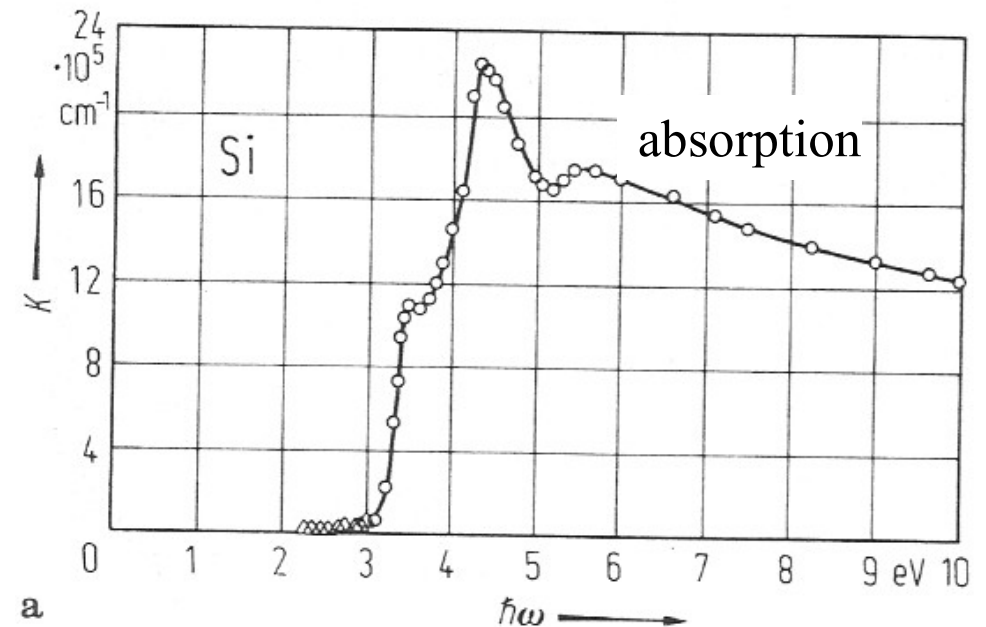
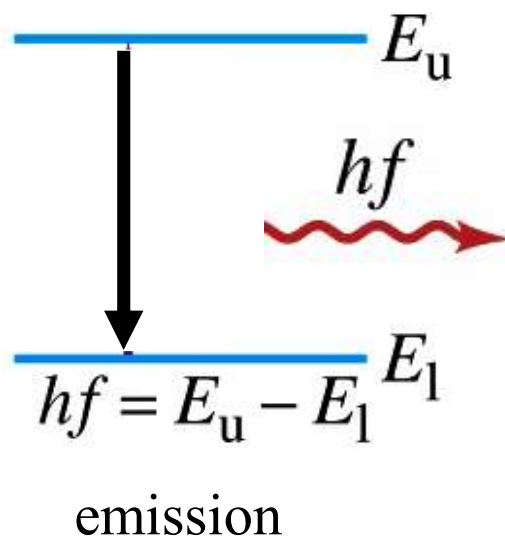
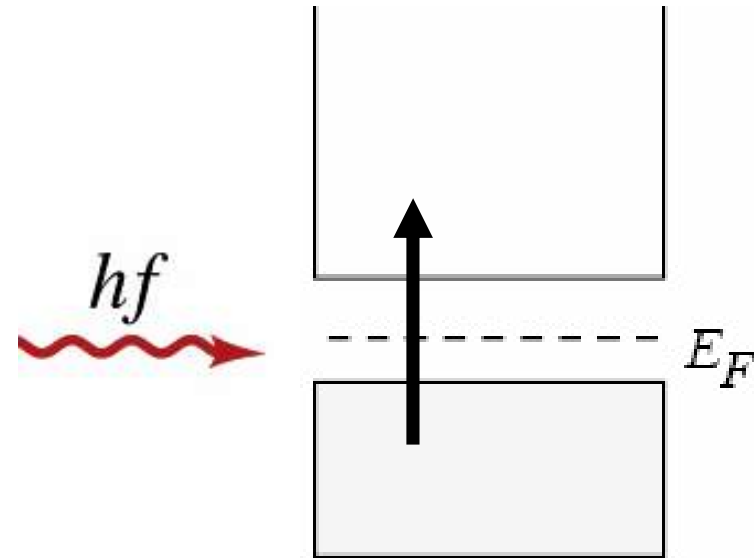
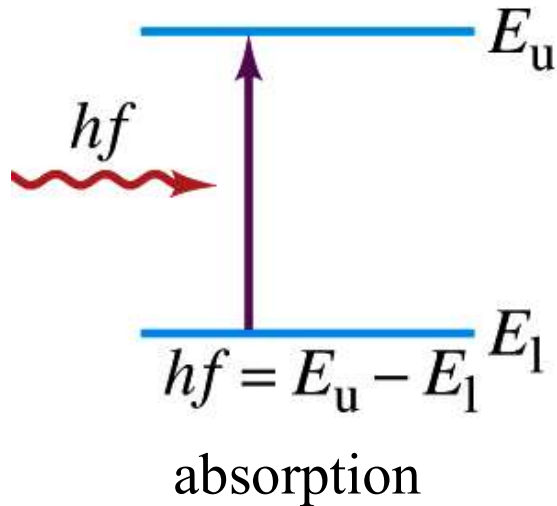
Semiconductors

Semiconductors

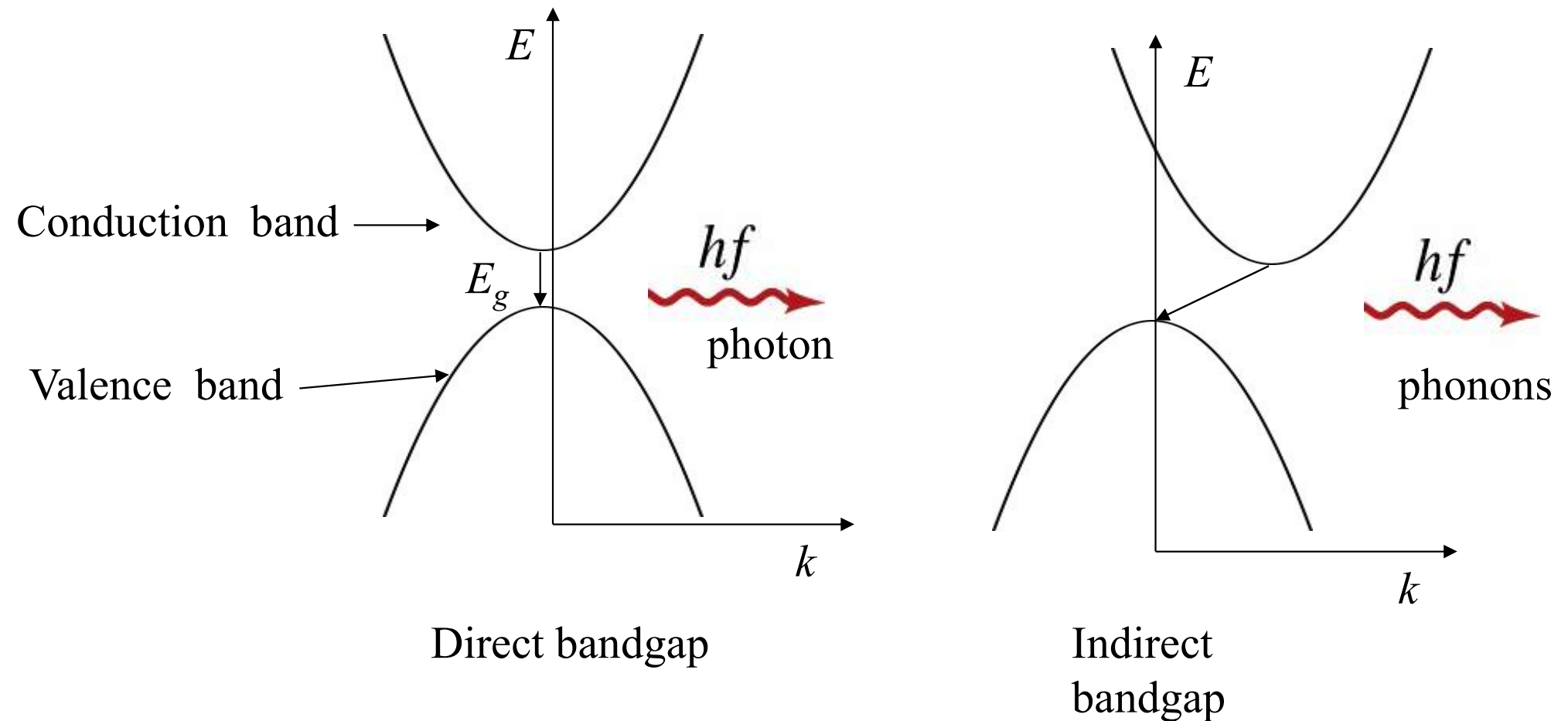


From Ibach & Lueth

Absorption and emission of photons

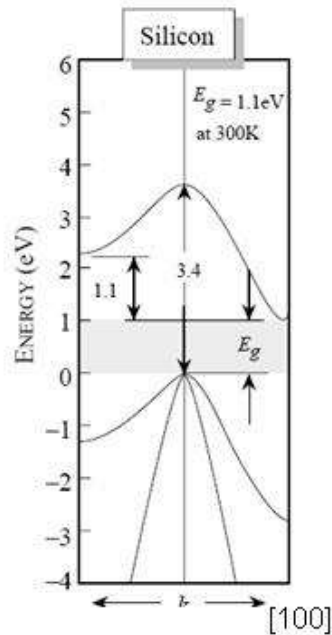


Direct and indirect band gaps

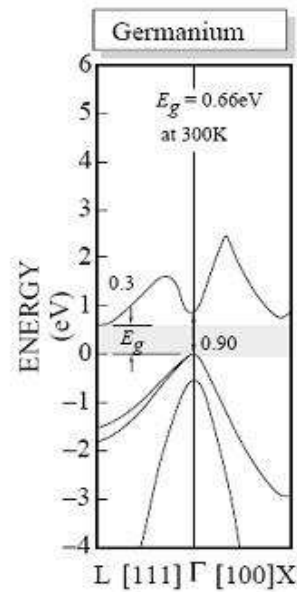


Direct bandgap semiconductors are used for optoelectronics

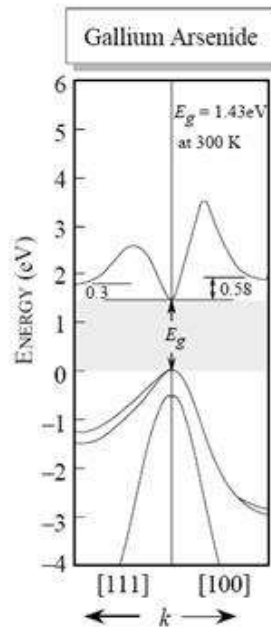
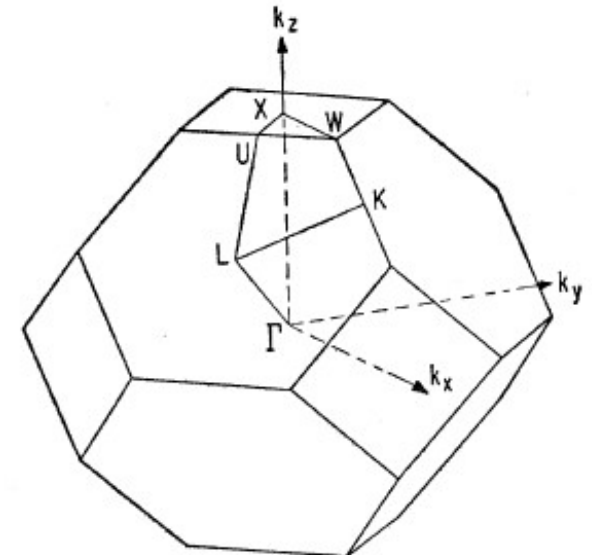
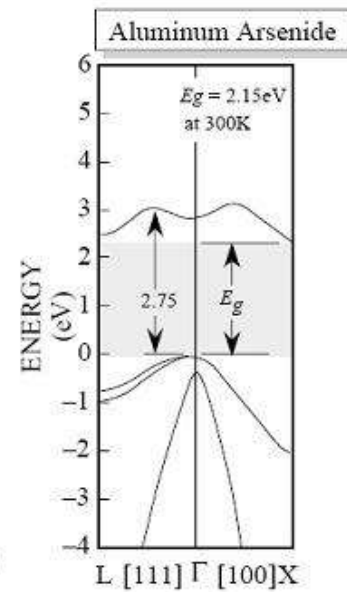
Semiconductors



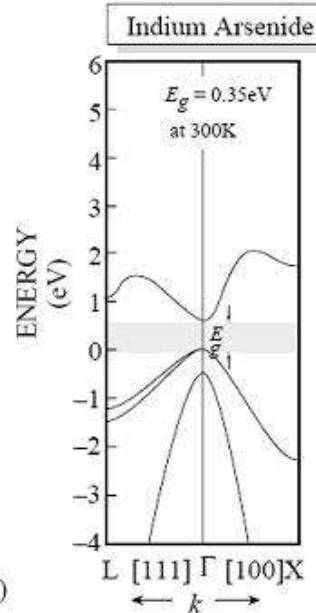
(a)



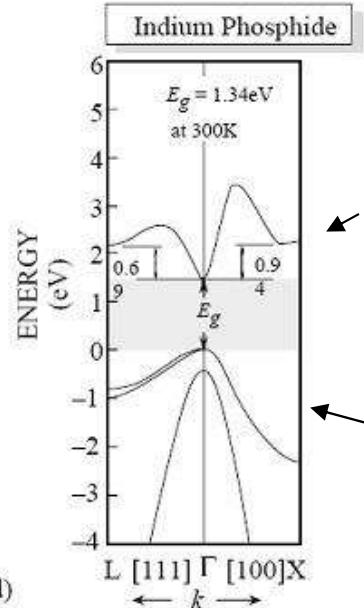
(b)



(c)



(d)



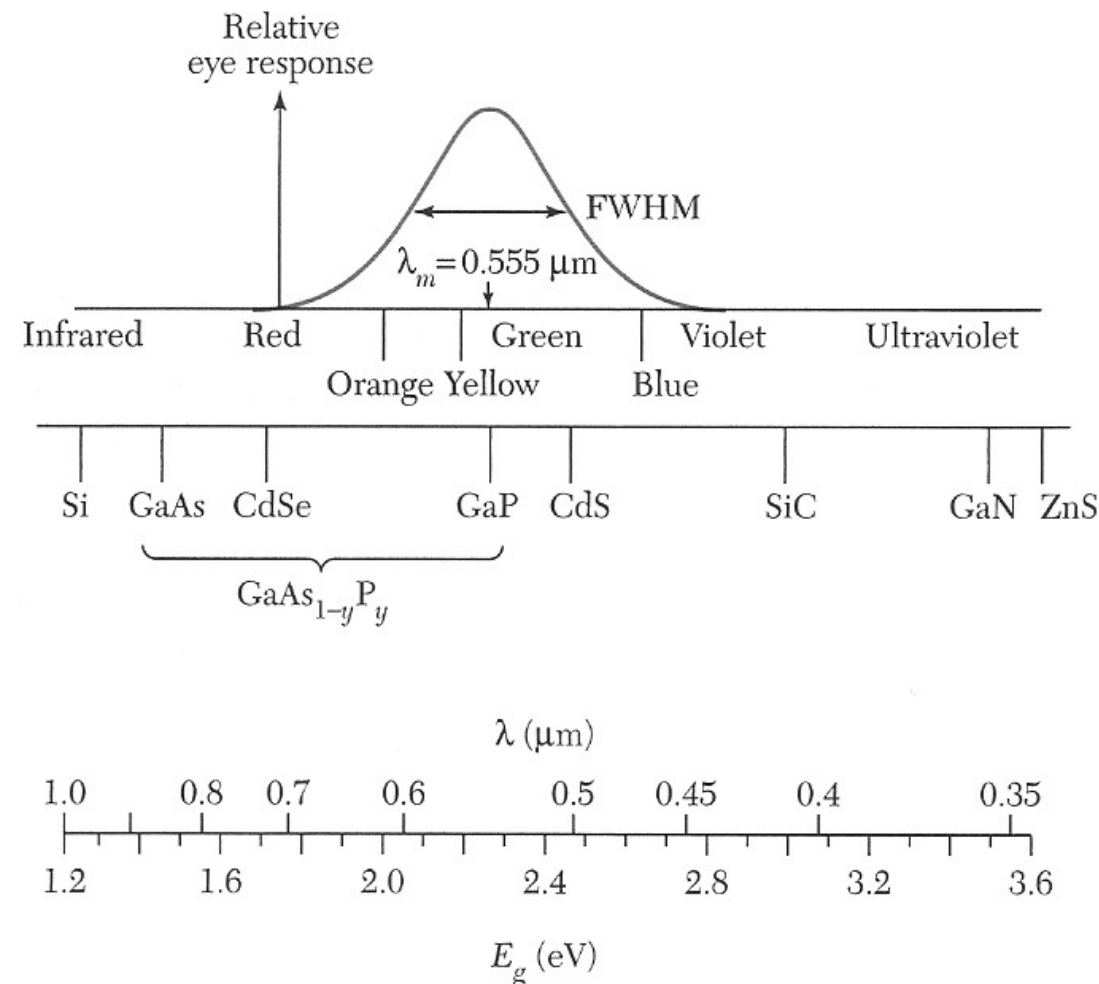
Conduction band

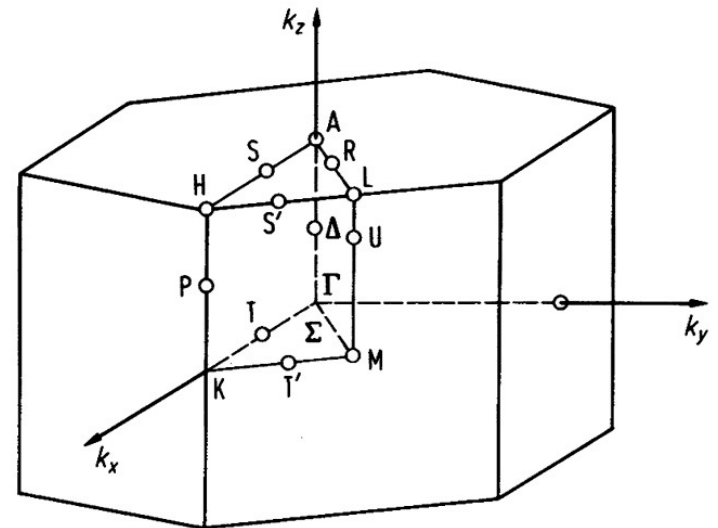
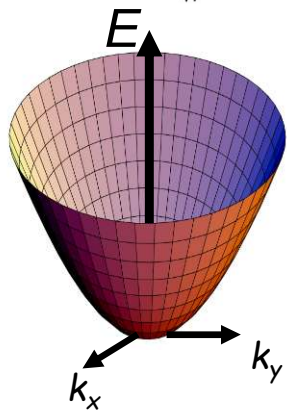
Valence band

TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$\text{Ga}_x\text{In}_{1-x}\text{As}_{1-y}\text{P}_y$	1100-1600
$\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$	1550
$\text{Ga}_{0.27}\text{In}_{0.73}\text{As}_{0.63}\text{P}_{0.37}$	1300
GaAs:Er, InP:Er	1540
Si:C	1300
GaAs:Yb, InP:Yb	1000
$\text{Al}_x\text{Ga}_{1-x}\text{As:Si}$	650-940
GaAs:Si	940
$\text{Al}_{0.11}\text{Ga}_{0.89}\text{As:Si}$	830
$\text{Al}_{0.4}\text{Ga}_{0.6}\text{As:Si}$	650
$\text{GaAs}_{0.6}\text{P}_{0.4}$	660
$\text{GaAs}_{0.4}\text{P}_{0.6}$	620
$\text{GaAs}_{0.15}\text{P}_{0.85}$	590
$(\text{Al}_x\text{Ga}_{1-x})_{0.5}\text{In}_{0.5}\text{P}$	655
GaP	690
GaP:N	550-570
$\text{Ga}_x\text{In}_{1-x}\text{N}$	340, 430, 590
SiC	400-460
BN	260, 310, 490

Light emitting diodes

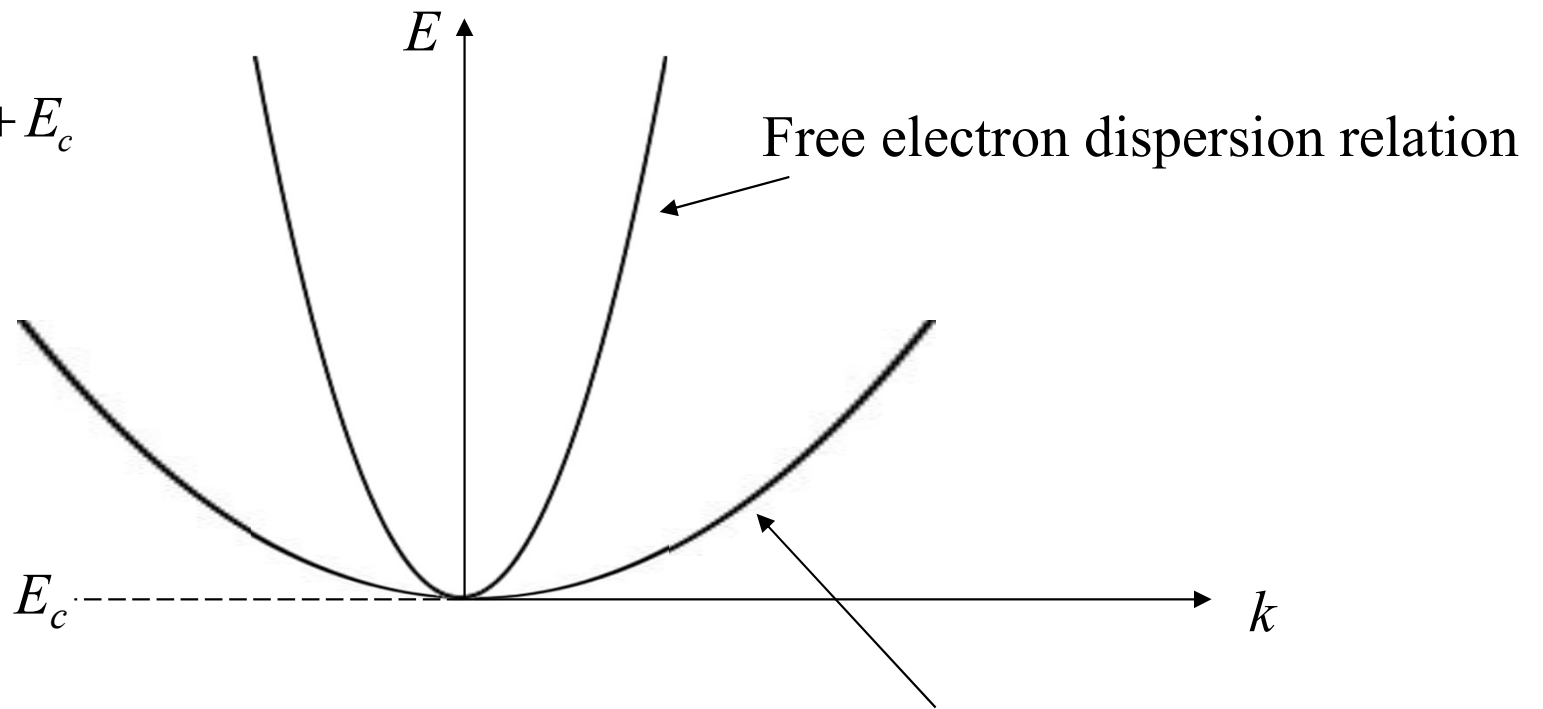




1st Brillouin zone of hcp

Conduction band minimum

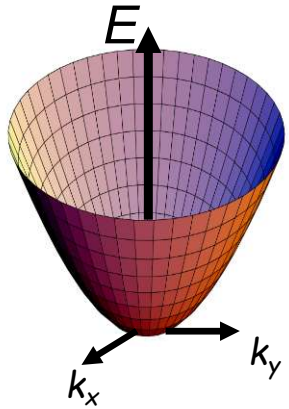
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*} + E_c$$



Minimum of the conduction band

Near the conduction band minimum, the bands are approximately parabolic.

Effective mass



$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*} + E_c$$

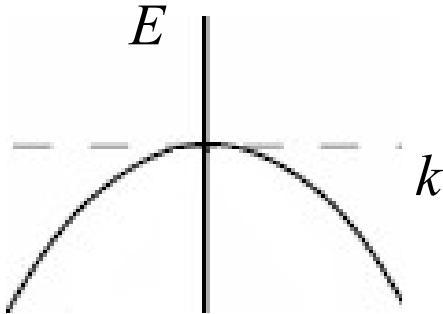
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

$$m^* = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

This effective mass is used to describe the response of electrons to external forces in the particle picture.

Top of the valence band

In the valence band, the effective mass is negative.



$$m^* = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}} < 0$$

Charge carriers in the valence band are positively charged holes.

m_h^* = effective mass of holes

$$m_h^* = \frac{-\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

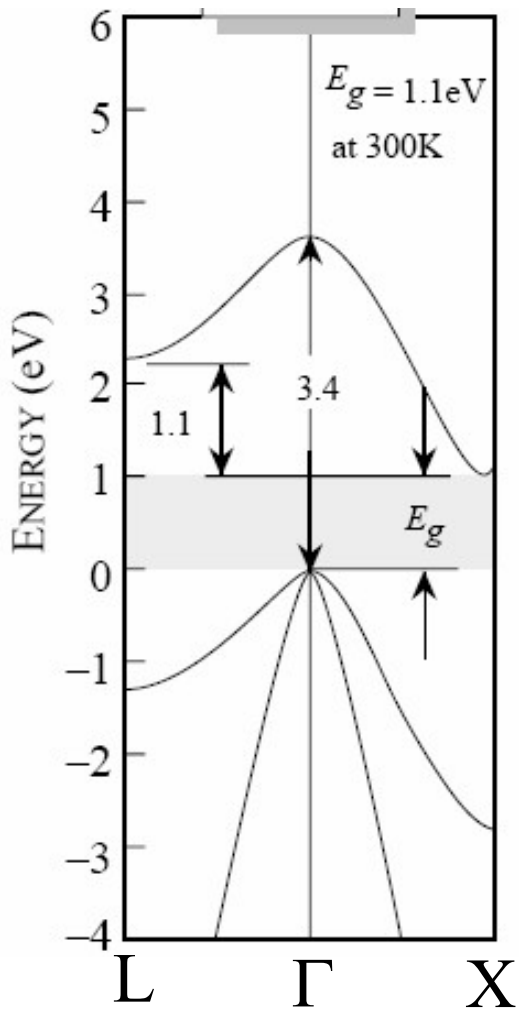
Holes

A completely filled band does not contribute to the current.

$$\begin{aligned}\vec{j} &= \int_{\text{filled states}} -e\vec{v}(\vec{k}) D(\vec{k}) d\vec{k} \\ &= \int_{\text{band}} -e\vec{v}(\vec{k}) D(\vec{k}) d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k}) D(\vec{k}) d\vec{k} \\ &= \int_{\text{empty states}} e\vec{v}(\vec{k}) D(\vec{k}) d\vec{k}\end{aligned}$$

Holes have a positive charge and a positive mass.

Effective Mass



$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*} + E_c$$

$$E = \frac{-\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*} + E_v$$

$$m_e^* = \frac{\hbar^2}{\frac{d^2 E}{dk_x^2}}$$

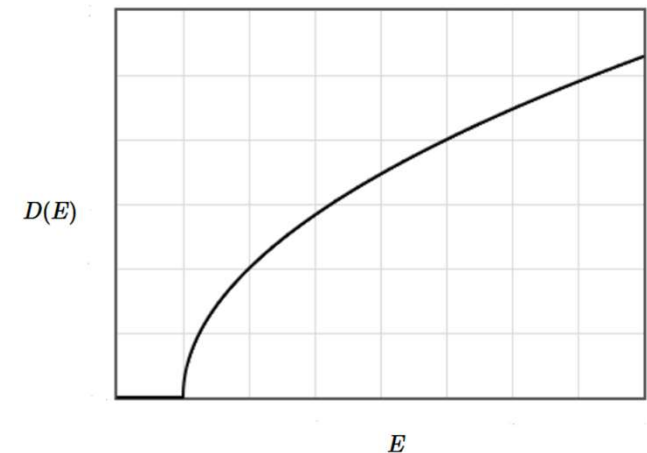
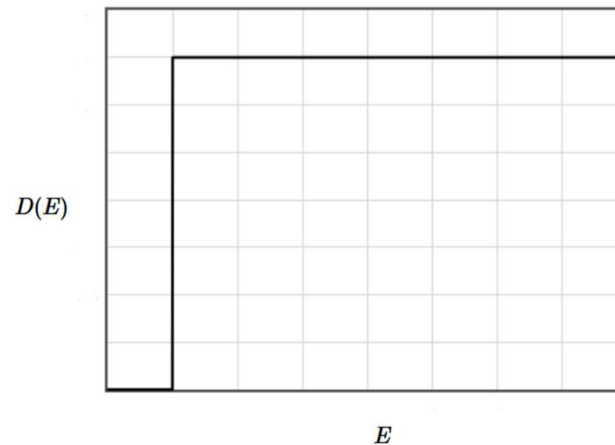
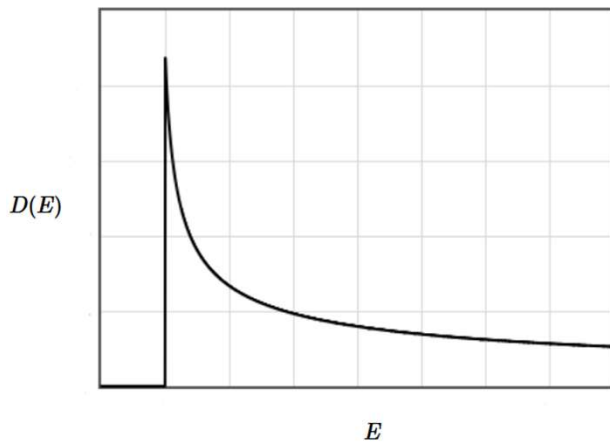
$$m_h^* = \frac{-\hbar^2}{\frac{d^2 E}{dk_x^2}}$$

Free electron Fermi gas

$$1 - d \quad D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1} \text{m}^{-1}$$

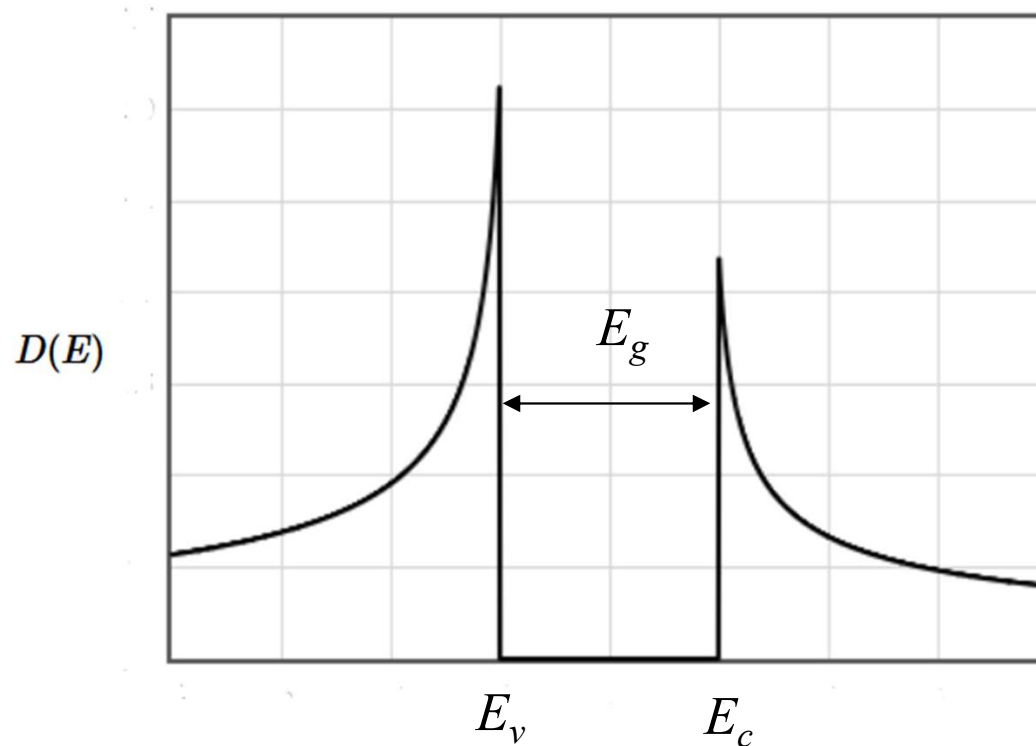
$$2 - d \quad D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1} \text{m}^{-2}$$

$$3 - d \quad D(E) = \frac{\pi}{2} \left(\frac{2m}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \text{J}^{-1} \text{m}^{-3}$$

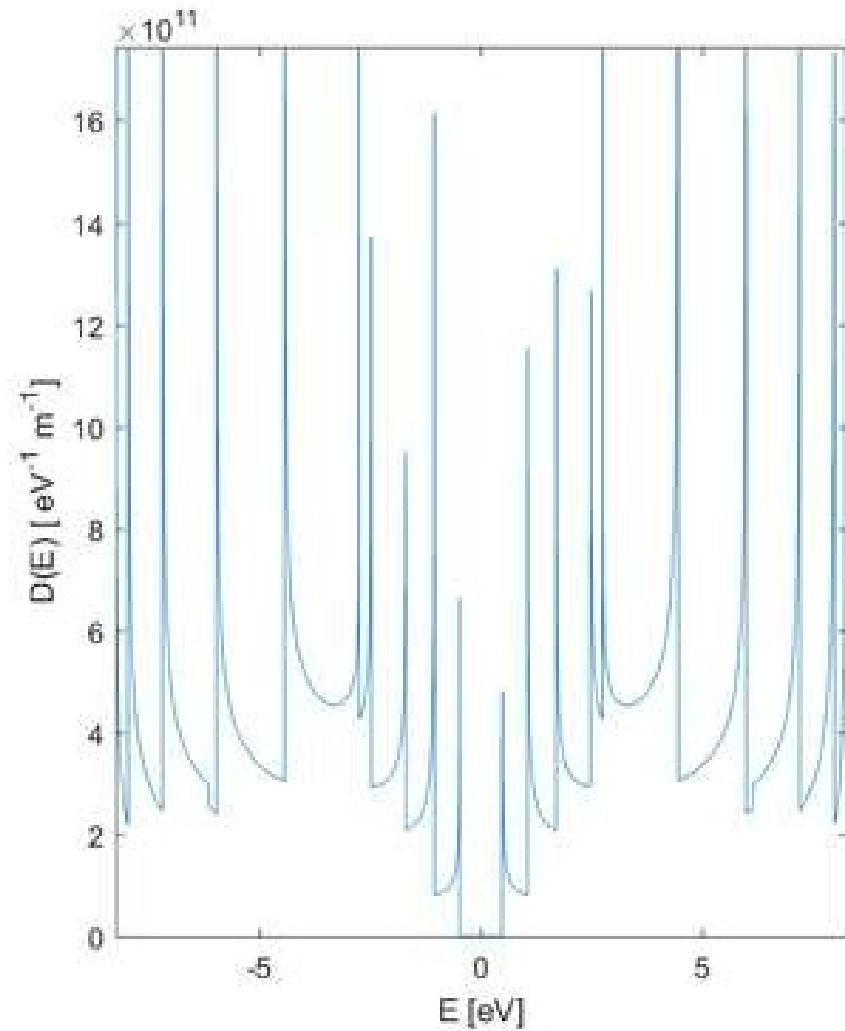
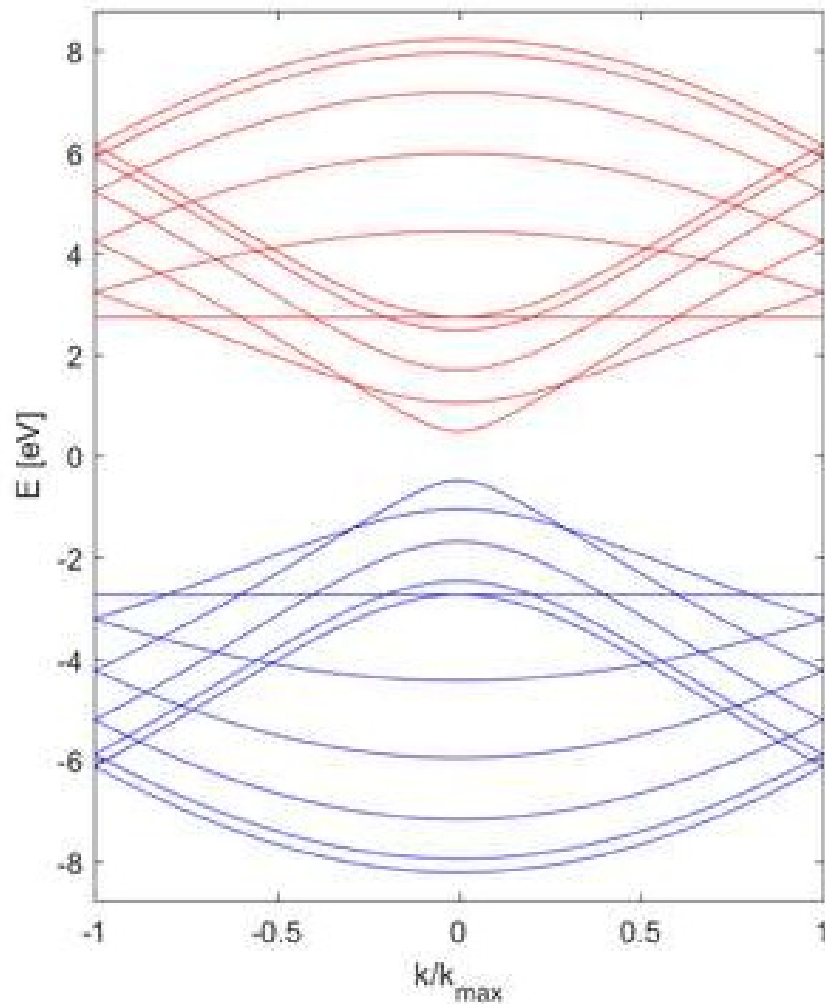


Semiconductors and insulators - 1d

$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$
$$D(E) = \begin{cases} \frac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

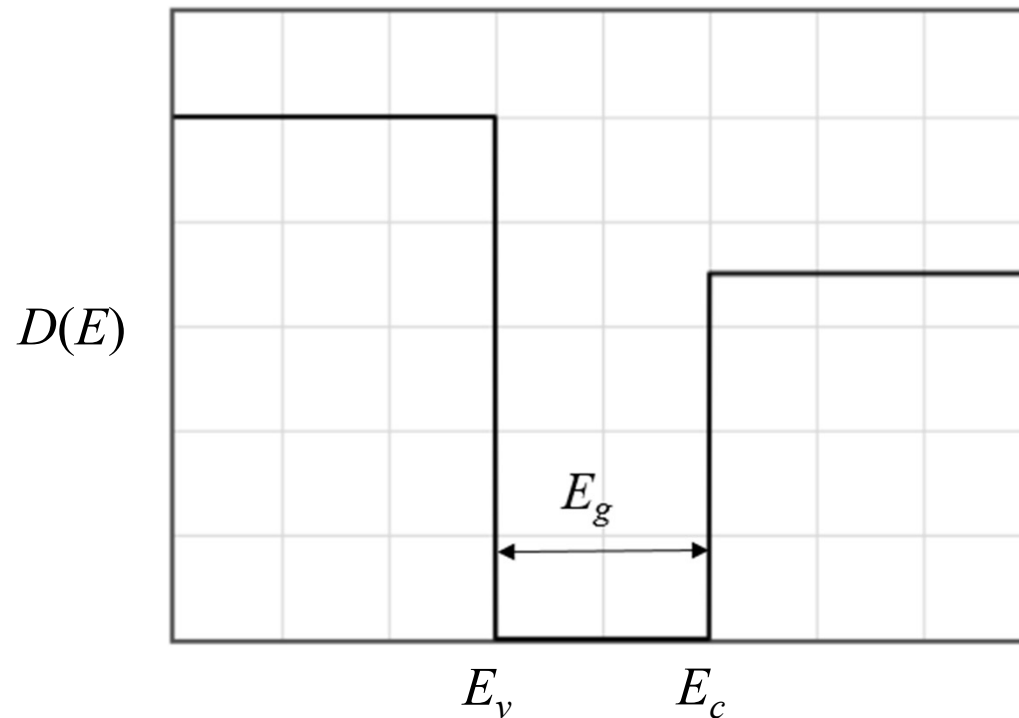


Semiconducting carbon nanotubes



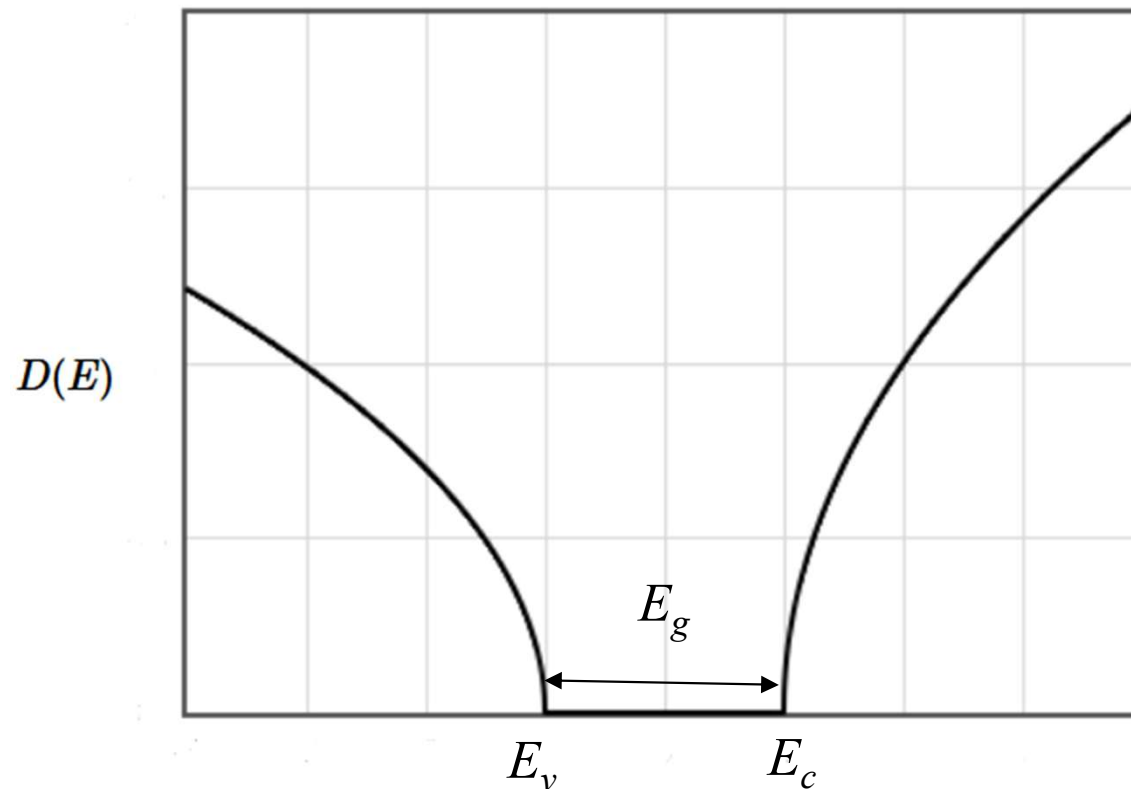
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

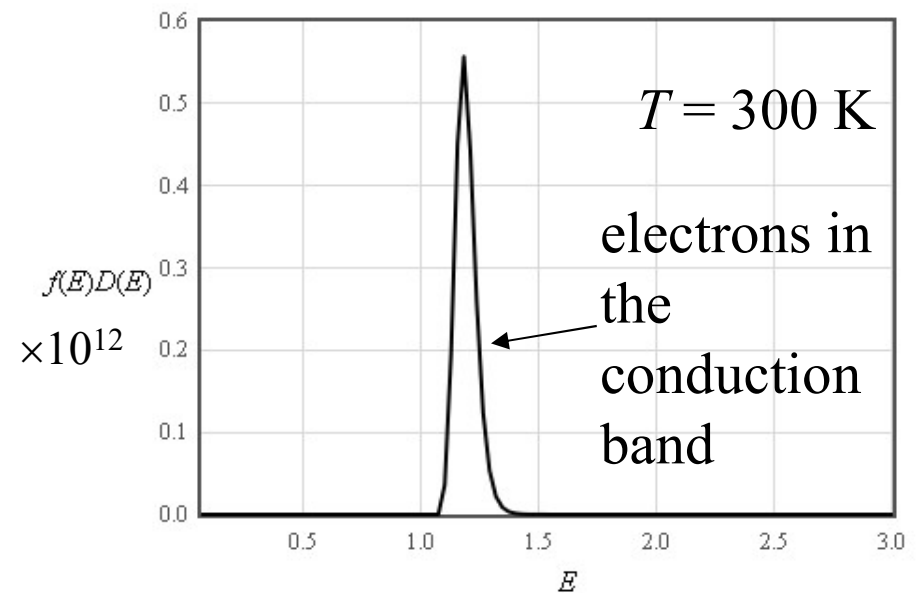
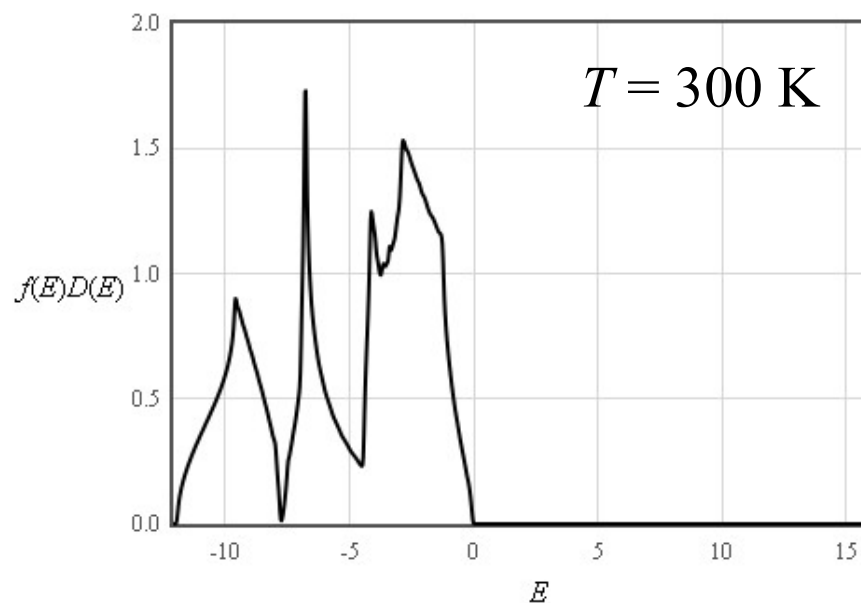
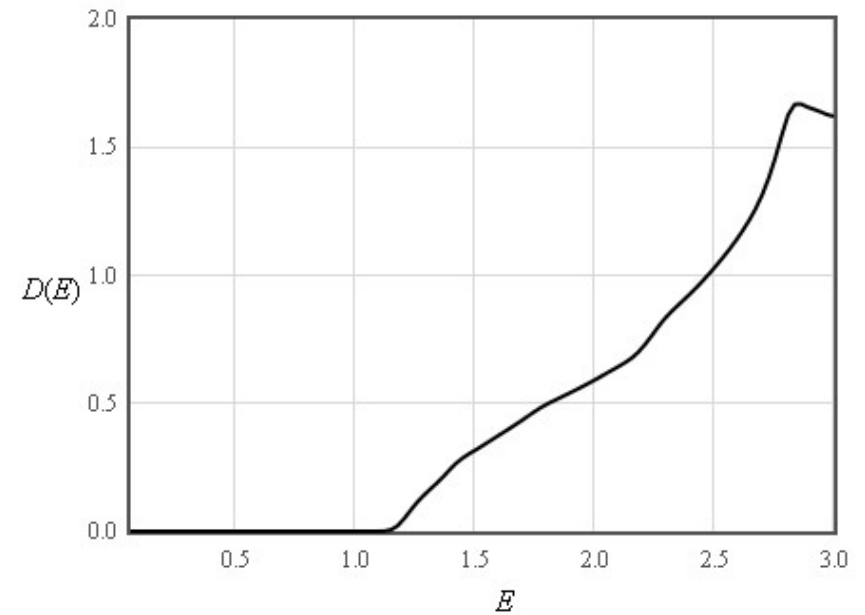
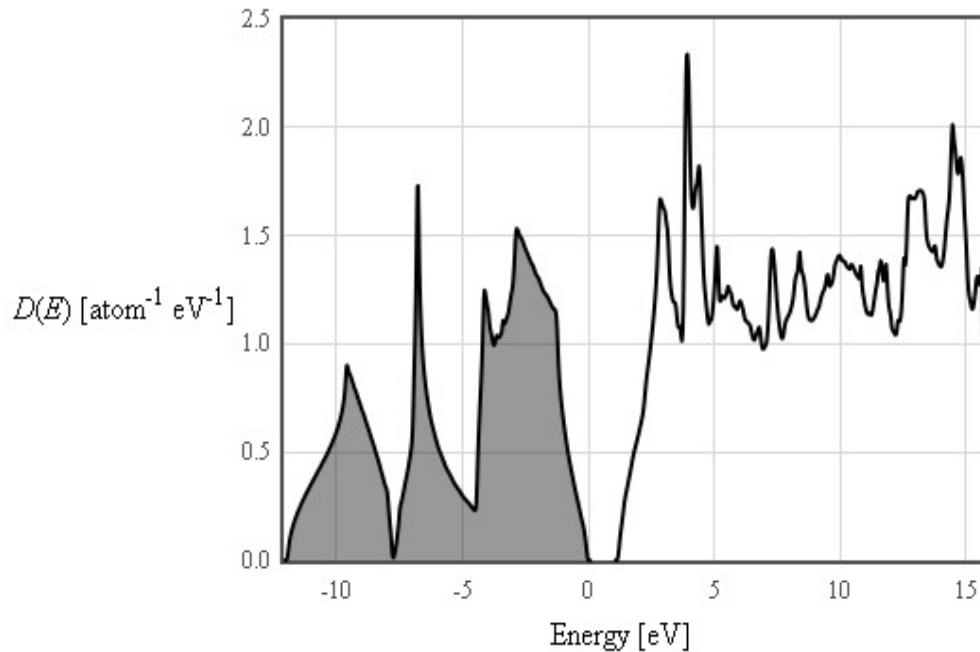


Semiconductors and insulators - 3d

$$D(E) = \begin{cases} D_v \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ D_c \sqrt{E - E_c} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



Silicon density of states



Boltzmann Approximation

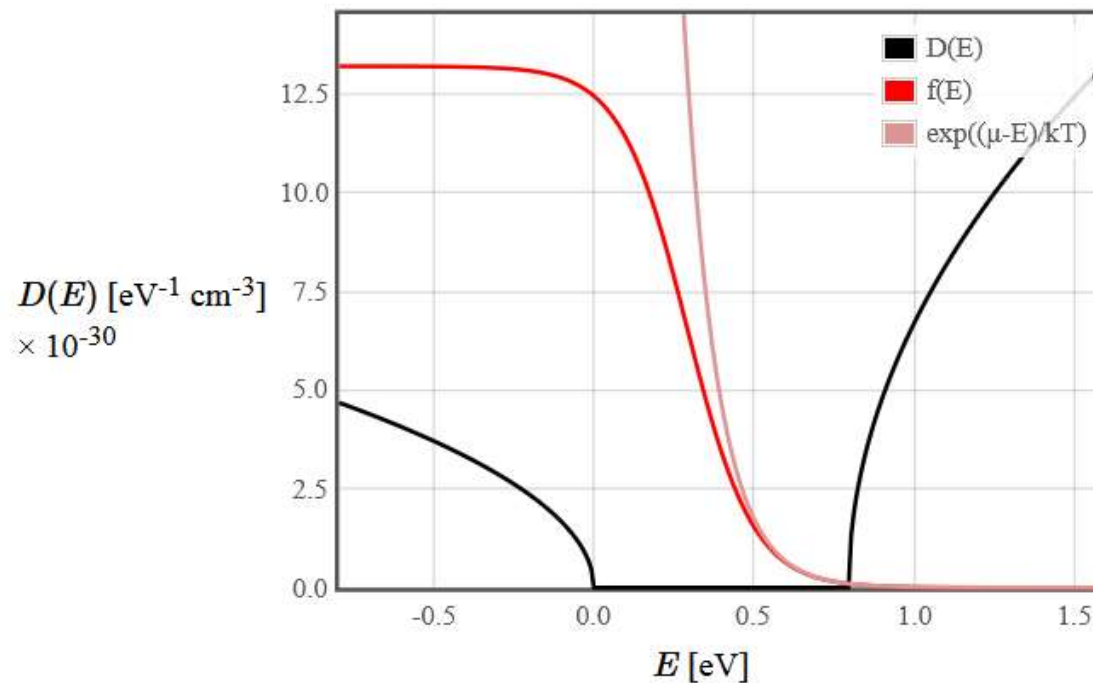
Density of electrons in the conduction band

The free electron density of states is modified by the effective mass.

$$D(E) = D_c \sqrt{E - E_c}$$

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{\mu - E}{k_B T}\right)$$

Boltzmann
approximation
 $E_c - \mu > 3k_B T$



$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$

Density of electrons in the conduction band

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$
$$= D_c \exp\left(\frac{\mu - E_c}{k_B T}\right) \int_{E_c}^{\infty} \exp\left(-\frac{E - E_c}{k_B T}\right) \sqrt{E - E_c} dE$$

$$x = E - E_c \quad \int_0^{\infty} \sqrt{x} \exp\left(\frac{-x}{k_B T}\right) dx = \frac{2}{\sqrt{\pi}} (k_B T)^{3/2}$$

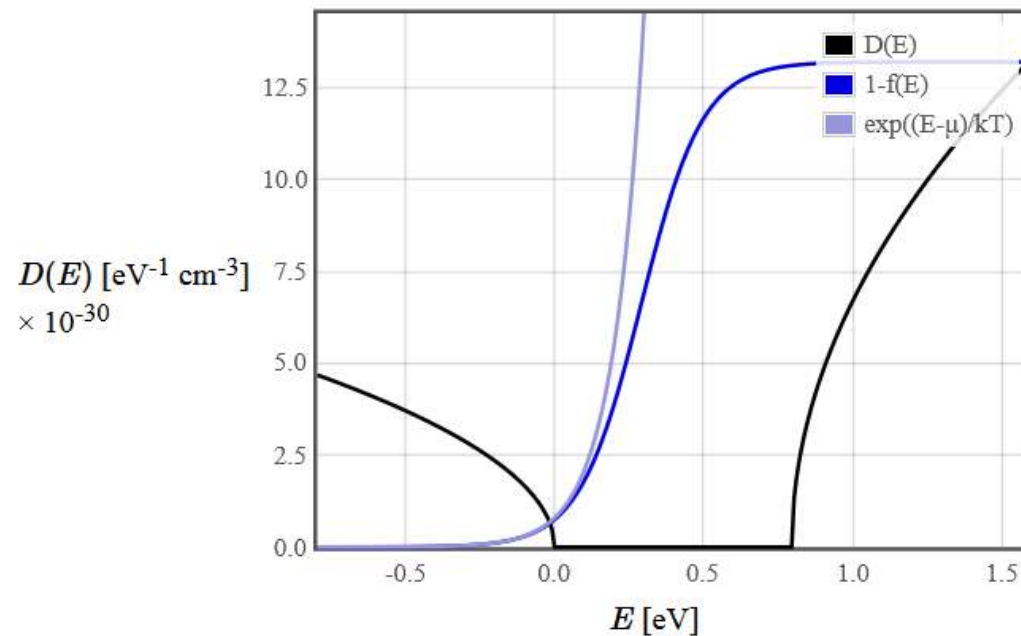
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{\sqrt{\pi} D_c}{2} (k_B T)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$$N_c = \frac{\sqrt{\pi} D_c}{2} (k_B T)^{3/2} = 2 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} = \text{effective density of states}$$

Density of holes in the valence band

$$D(E) = D_v \sqrt{E_v - E}$$

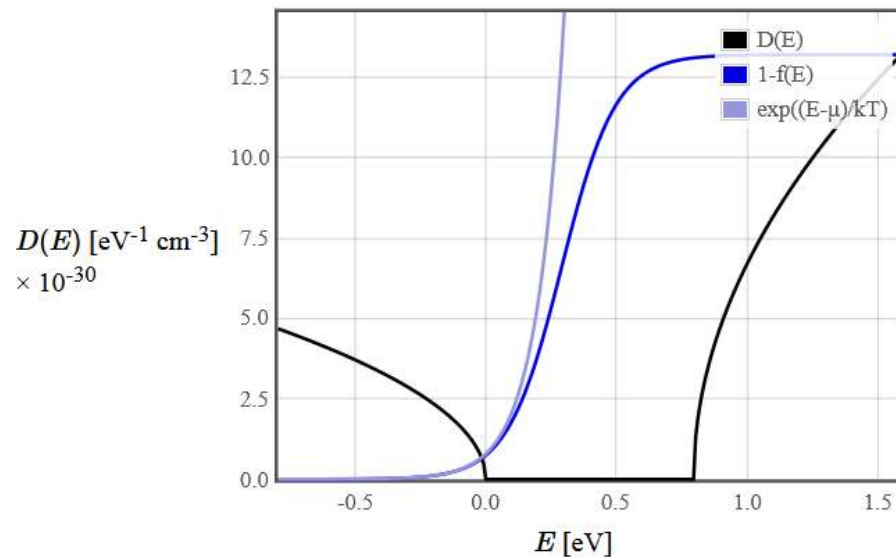
$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{E - \mu}{k_B T}\right)$$



Boltzmann
approximation
 $\mu - E_v > 3k_B T$

$$p = \int_{-\infty}^{E_v} D(E)(1 - f(E)) dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E} dE$$

Density of holes in the valence band



$$p = \int_{-\infty}^{E_v} D(E)(1-f(E)) dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right) \sqrt{E_v-E} dE$$

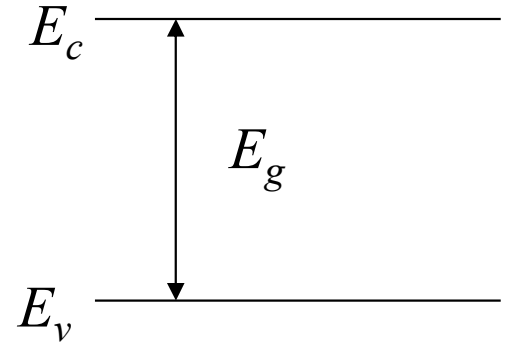
$$p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right) = \frac{\sqrt{\pi} D_v}{2} (k_B T)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$N_v = 2 \left(\frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} = \text{Effective density of states in the valence band}$$

Law of mass action

$$np = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

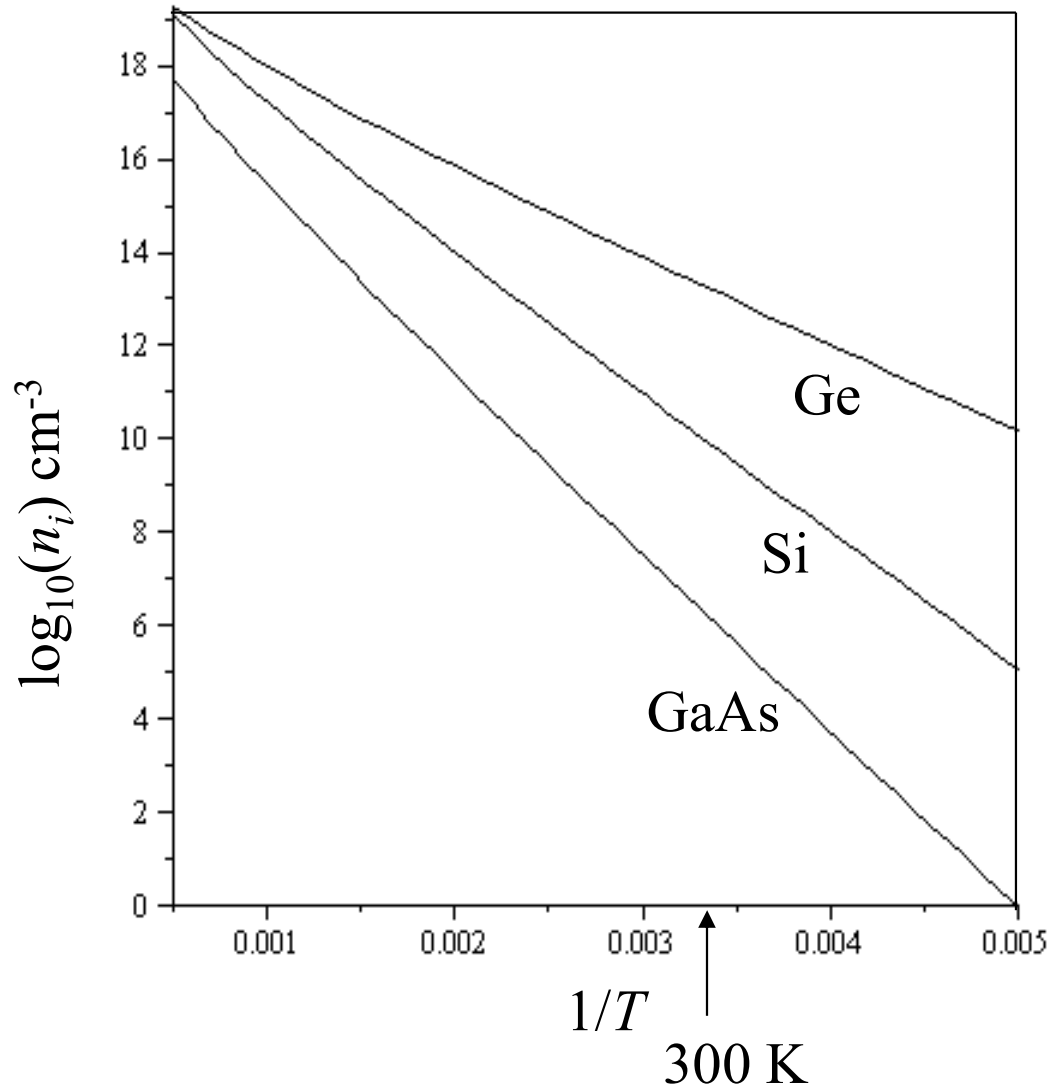


For intrinsic semiconductors (no impurities)

$$n = p = n_i = \sqrt{N_c N_v} \exp\left(\frac{-E_g}{2k_B T}\right)$$

intrinsic carrier density

Intrinsic carrier concentration



$$n_i = \sqrt{N_v N_c \left(\frac{T}{300} \right)^3} \exp \left(-\frac{E_g}{2k_B T} \right)$$

$$\sim 5 \times 10^{22} \text{ atoms/cm}^3$$

Chemical potential of an intrinsic semiconductor

$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$\exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right) = \frac{N_v}{N_c}$$

$$\frac{2\mu}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

$$\boxed{\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)}$$

E_c _____

μ -----

E_v _____

Boltzmann approximation

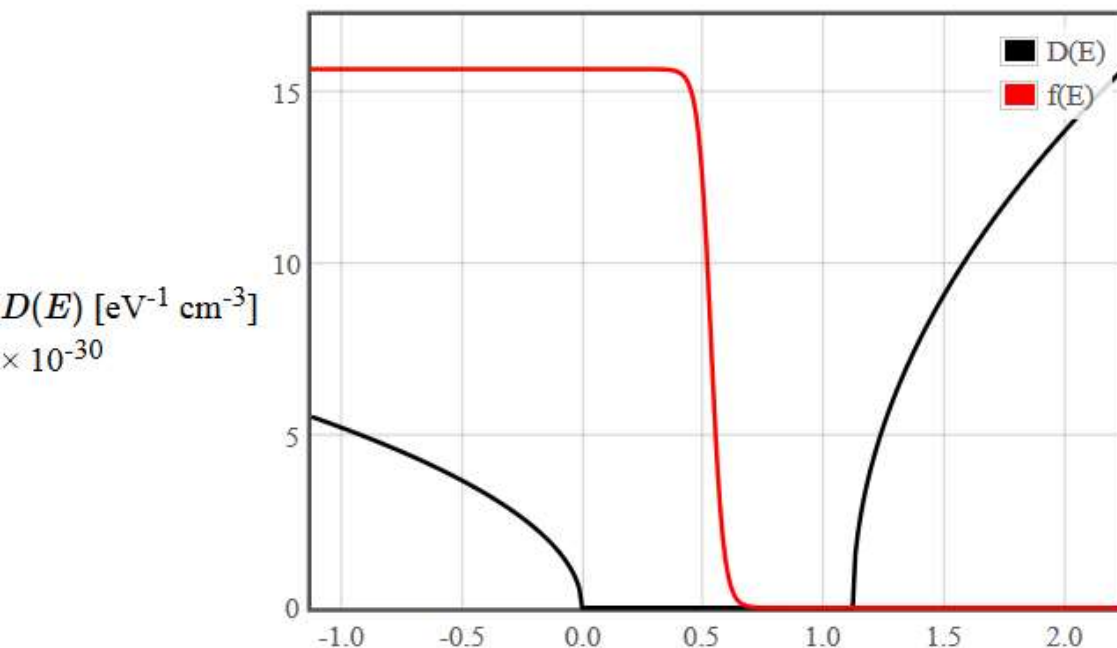
of the valence band and the bottom of the conduction band the density of states of a semiconductor can be approximated as,

$$D(E) = \begin{cases} D_v \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

and D_c are constants that describe the form of the density of states near the band edges. Often in the literature, these constants are given in terms of the masses' m_h^* and m_e^* or the 'effective density of states at 300 K' $N_v(300)$ and $N_c(300)$. The relations to D_v and D_c are,

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2 \hbar^3} = \frac{\sqrt{\pi} N_v(300)}{2(k_B T)^{3/2}}, \quad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2 \hbar^3} = \frac{\sqrt{\pi} N_c(300)}{2(k_B T)^{3/2}}.$$

ow shows the density of states of various semiconductors in this approximation. The Fermi function is plotted as well. At low energies the value of the states are occupied. At high energies the Fermi function goes to zero and those states are unoccupied. In the limit of low temperature, the chemical potential $\mu = E_g/2$. As the temperature increases, the chemical potential moves towards the band with the lower density of states.



$D_c =$	1.48E31	1/eV 1/cm ³
$D_v =$	5.25E30	1/eV 1/cm ³
$E_g =$	1.166-4.73E-4*T*T/(T+636)	eV
$T_1 =$	300	K
Replot		

Semiconductor		
Si	Ge	GaAs
InAs	InP	InSb

The electrical contribution to the thermodynamic properties of insulators depend on band edges

Boltzmann approximation

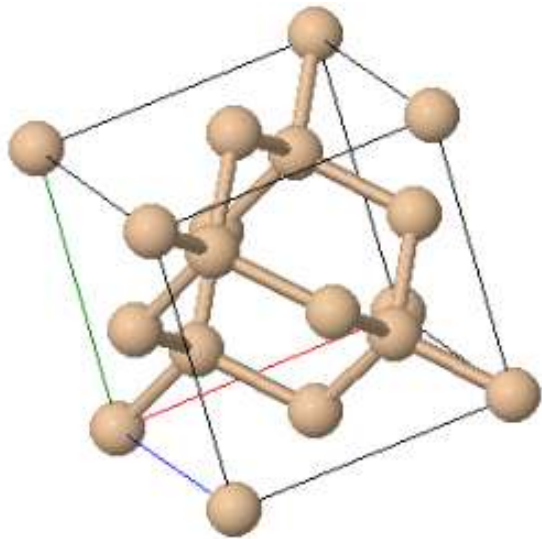
The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results were calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_B T$ from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

	1-d	2-d
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{ m}^{-1}$	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{ m}^{-2}$ $H(x) = 0 \text{ for } x < 0 \text{ and } H(x) = 1 \text{ for } x > 0$
Density of states N_v and N_c are the effective densities of states	$D(E) = \begin{cases} N_v(300) \sqrt{\frac{2}{300\pi k_B (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300) \sqrt{\frac{2}{300\pi k_B (E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{ m}^{-1}$	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{N_c(300)}{300k_B} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{ m}^{-2}$
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-1}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-2}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-1}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-2}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

Silicon

- Important semiconducting material
- 2nd most common element on earth's crust (rocks, sand, glass, concrete)
- Often doped with other elements
- Oxide SiO_2 is a good insulator

2.33		28.086
	Si	14
5.43	$3s^2 3p^2$	
1683	DIA	625



silicon crystal = diamond crystal structure

513.160 Microelectronics and Micromechanics

Silicon

Silicon is the second most common element in the earth's crust and an important semiconducting material.

Structural properties

Crystal structure: Diamond

Bravais lattice: face centered cubic

Space group: 227 (F d -3 m), Strukturbericht: A4, Pearson symbol: cF8

Point group: m3m (O_h) six 2-fold rotations, four 3-fold rotations, three 4-fold rotations, nine mirror planes, inversion

Lattice constant: $a = 0.357 \text{ nm}$

Atomic weight 28.09

Atomic density $n_{atoms} = 4.995 \times 10^{22} \text{ 1/cm}^3$

Density $\rho = 2.33 \text{ g/cm}^3$

Density of surface atoms

(100) $6.78 \times 10^{14} \text{ 1/cm}^2$

(110) $9.59 \times 10^{14} \text{ 1/cm}^2$

(111) $7.83 \times 10^{14} \text{ 1/cm}^2$

HM: F d -3 m S

$a=5.430 \text{ \AA}$

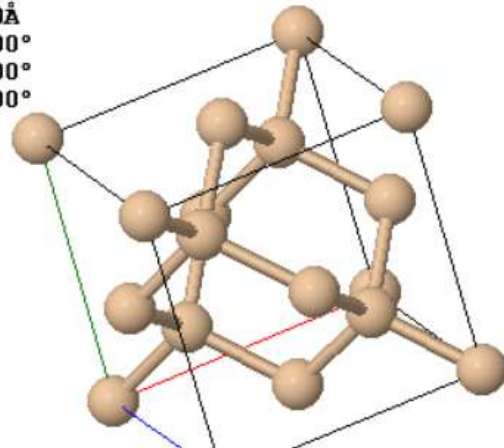
$b=5.430 \text{ \AA}$

$c=5.430 \text{ \AA}$

$\alpha=90.000^\circ$

$\beta=90.000^\circ$

$\gamma=90.000^\circ$



Conventional unit cell

Primitive unit cell

Asymmetric unit

2 x 2 x 2

3 x 3 x 3

5 x 5 x 5

Ball and Stick

Spacefill

H: 1

K: 0

L: 0

show HKL plane

hide HKL plane

draw atoms in HKL plane

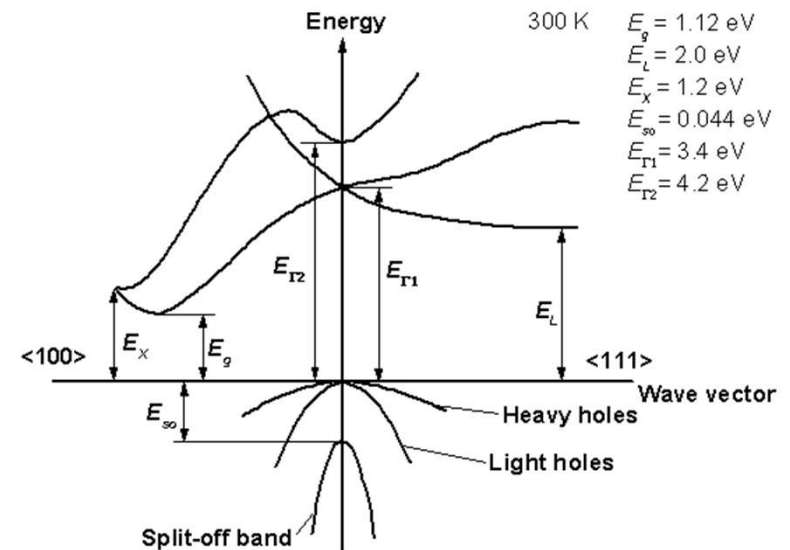
Thickness of HKL planes:

The conventional unit cell is a cube with sides of 0.357 nm. There are 8 atoms in the conventional unit cell. (The

Semiconductors	n,k
database	InGaAsP Levels Equivalents Bibliografic database

NSM Archive - Physical Properties of Semiconductors

Si	- Silicon	Ge	- Germanium
GaP	- Gallium Phosphide	GaAs	- Gallium Arsenide
InAs	- Indium Arsenide	C	- Diamond
GaSb	- Gallium Antimonide	InSb	- Indium Antimonide
InP	- Indium Phosphide	GaAs _{1-x} Sb _x	- Gallium Arsenide Antimonide
Al _x Ga _{1-x} As	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride		
BN	- Boron Nitride		



<http://www.matprop.ru/semicond>

Intrinsic semiconductors

In the Boltzmann approximation, the density of states of a semiconductor is,

$$D(E) = \begin{cases} \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} \sqrt{E_v - E}, & \text{if } E < E_v \\ 0, & \text{if } E_v < E < E_c \\ \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \sqrt{E - E_c}, & \text{if } E_c < E \end{cases}$$

Here m_e^* and m_h^* are the 'density of states effective masses' for electrons and holes. Usually in the literature, effective density of states at 300 K is given instead of the 'density of states effective masses'. The relationship between the two is,

$$m_h^* = \frac{\pi\hbar^2}{300k_B} \left(\sqrt{2}N_v(300) \right)^{2/3}$$

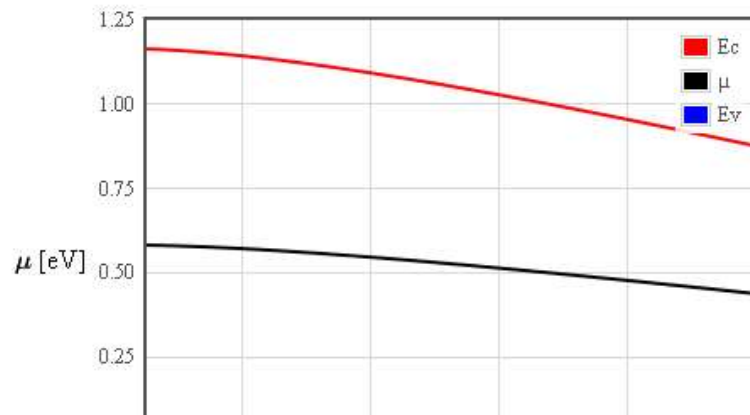
$$m_e^* = \frac{\pi\hbar^2}{300k_B} \left(\sqrt{2}N_c(300) \right)^{2/3}$$

In an intrinsic semiconductor, the density of electrons equals the density of holes, $n = p = n_i = \sqrt{N_c \left(\frac{T}{300} \right)^{3/2} N_v \left(\frac{T}{300} \right)^{3/2} \exp\left(\frac{-E_g}{2k_B T} \right)}$.

By setting the concentration of electrons equal to the concentration of holes, it is possible to solve for the chemical potential. The bandgap of most semiconductors is temperature dependent. The form below lets you input the temperature dependence of the bandgap. The bandgaps for some semiconductors can be loaded into the form with the buttons on the right.

$$n = N_c(300) \left(\frac{T}{300} \right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T} \right) = p = N_v(300) \left(\frac{T}{300} \right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T} \right)$$

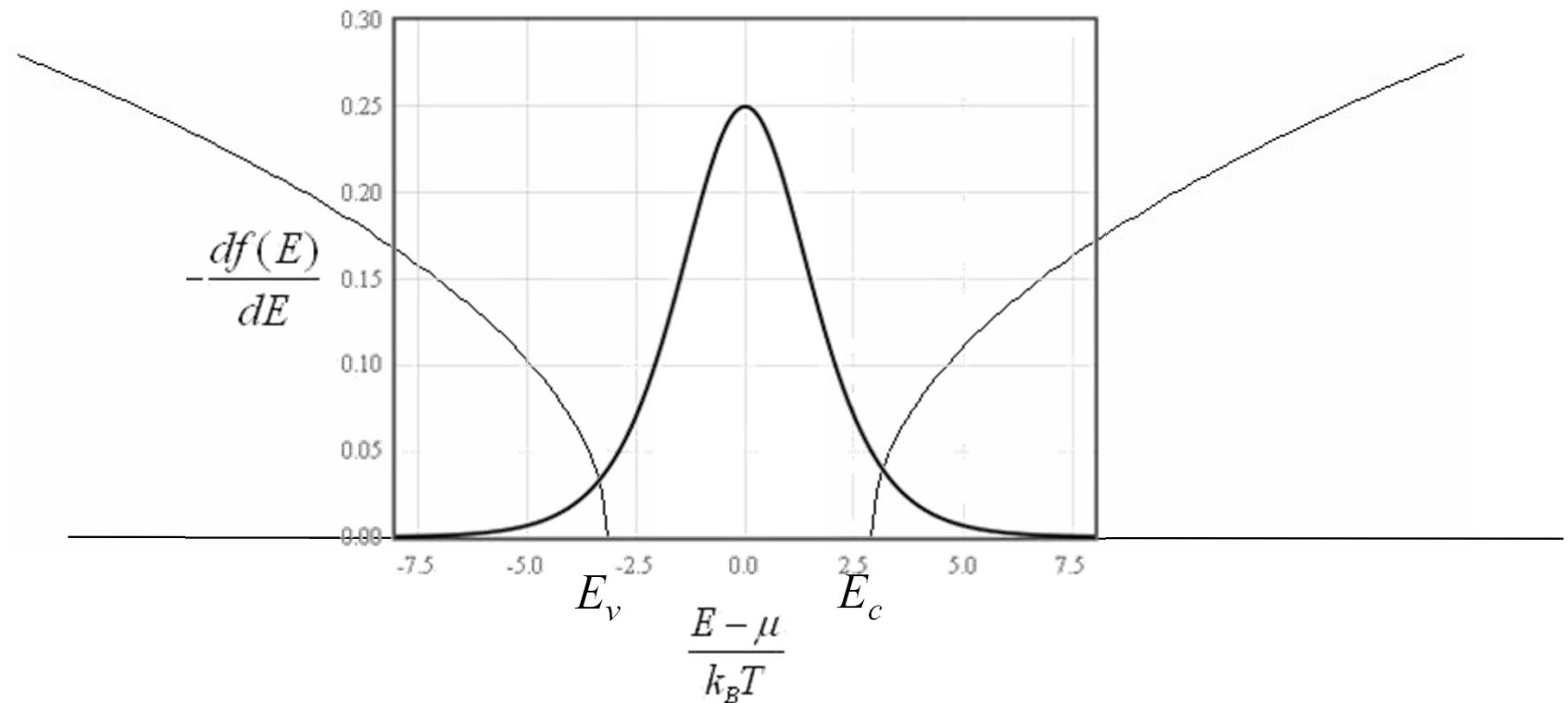
$$\mu = \frac{E_v + E_c}{2} + k_B T \ln\left(\frac{N_v(300)}{N_c(300)} \right)$$



$N_c(300 \text{ K}) =$	2.78E19	1/cm ³
$N_v(300 \text{ K}) =$	9.84E18	1/cm ³
$E_g =$	1.166-4.73E-4*T*(T+636)	eV
$T_1 =$	50	K
$T_2 =$	1000	K
Replot		

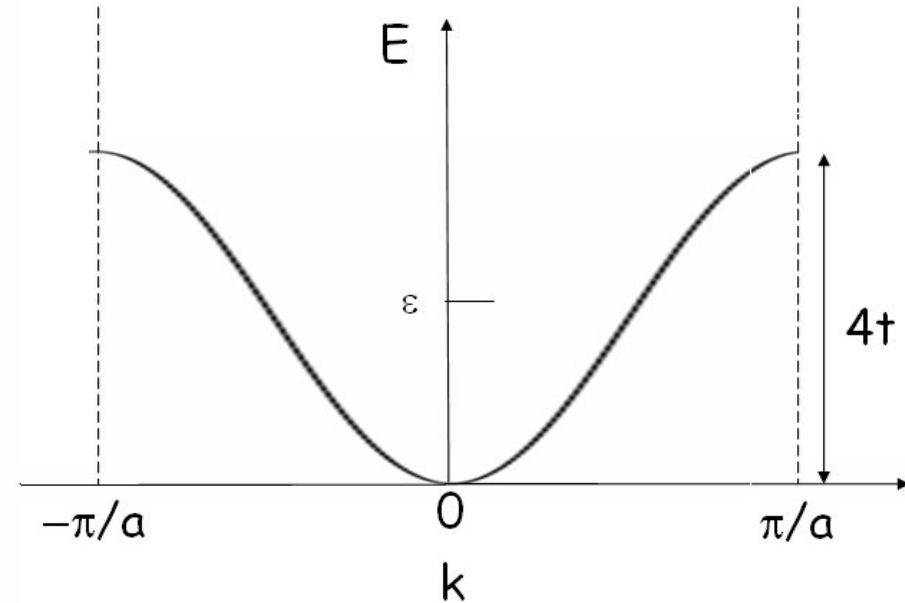
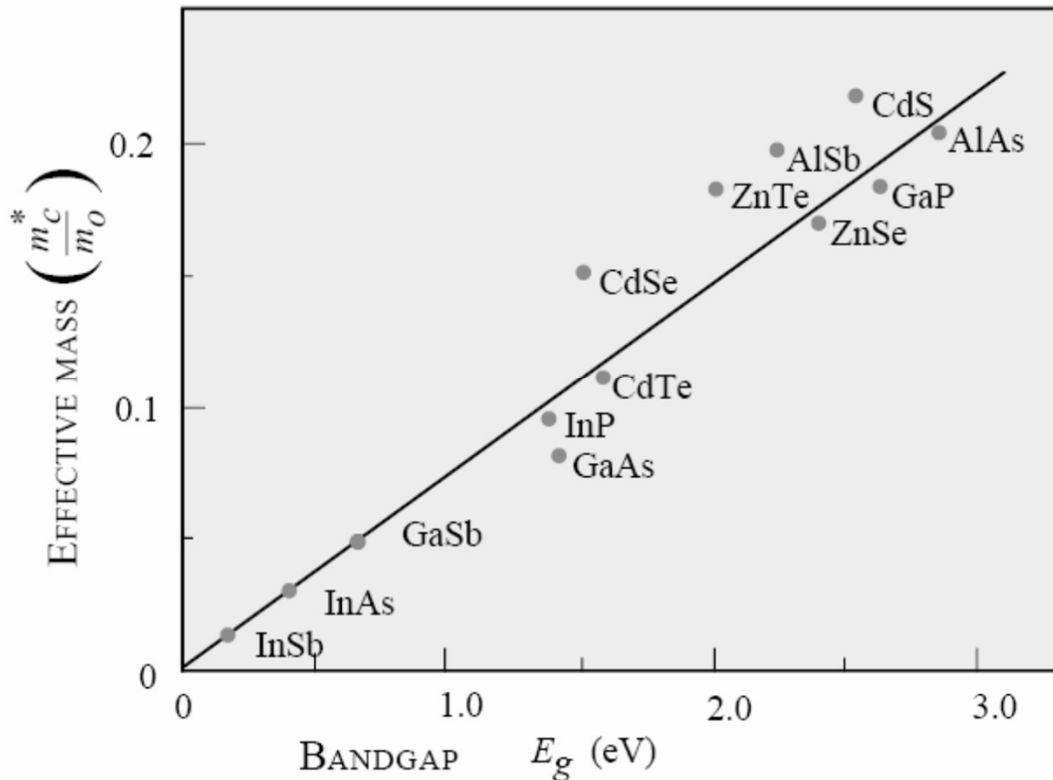
Semiconductor

Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

Large gap -> large effective mass



$$m^* = \frac{\hbar^2}{\frac{d^2 E}{dk^2}}$$

$$E_k = \varepsilon - 2t \cos(ka)$$

$$\frac{d^2 E}{dk^2} = 2ta^2$$

$$m^* \propto \frac{1}{t}$$

narrow bands -> large effective mass