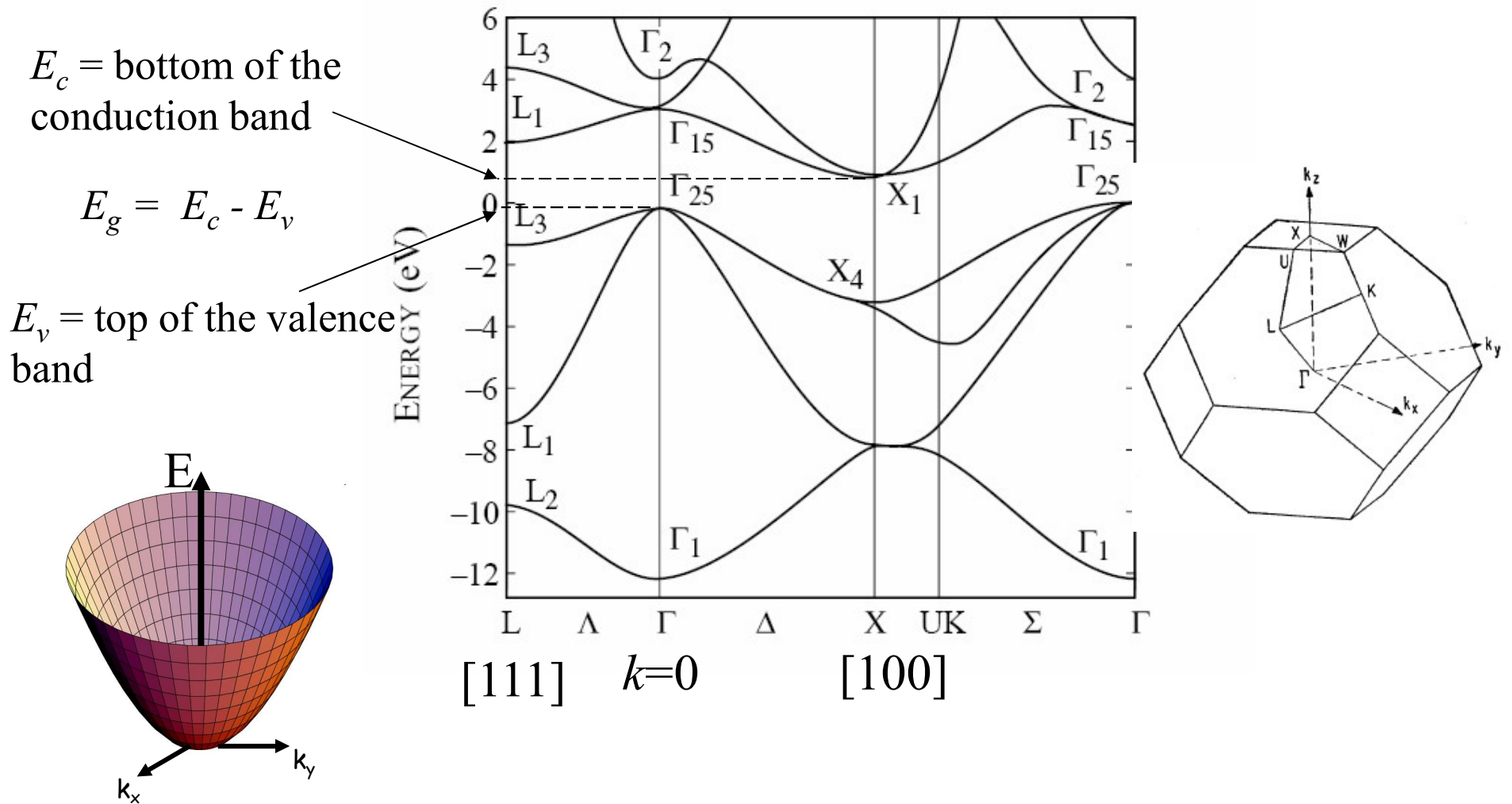


# Intrinsic semiconductors

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# Silicon band structure



Near the bottom of the conduction band, the band structure looks like a parabola.

# Effective mass

---

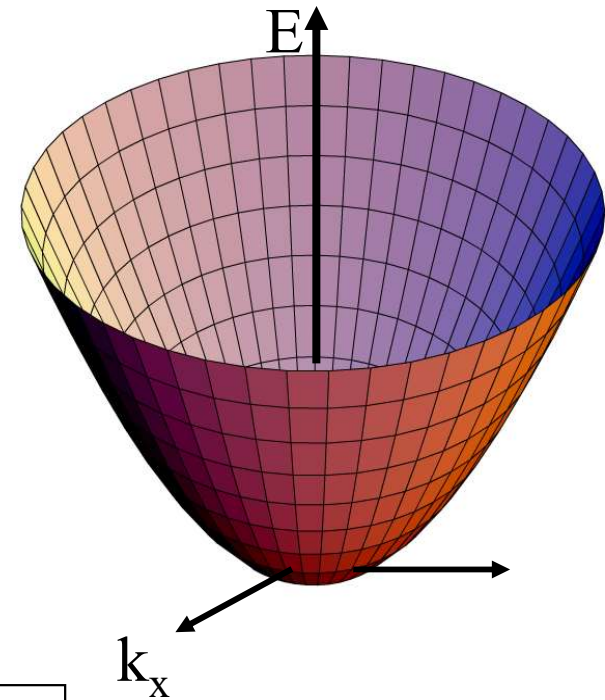
$$E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) = \frac{p^2}{2m} = \frac{1}{2} m v^2$$

$$\frac{dE(\vec{k})}{dk_x} = \frac{\hbar^2 k_x}{m}$$

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

Effective mass

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



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

$$\vec{F} = -e\vec{E} = m^* \vec{a}$$

# valence band, holes

---

When all states in a band are occupied, the band does not contribute to the current. There are as many left-moving electrons as right-moving electrons.

$$I \propto \sum_{\text{occupied } \vec{k}} (-e\vec{v}_{\vec{k}})$$

$$I \propto \sum_{\text{all } \vec{k}} (-e\vec{v}_{\vec{k}}) - \sum_{\text{empty } \vec{k}} (-e\vec{v}_{\vec{k}})$$

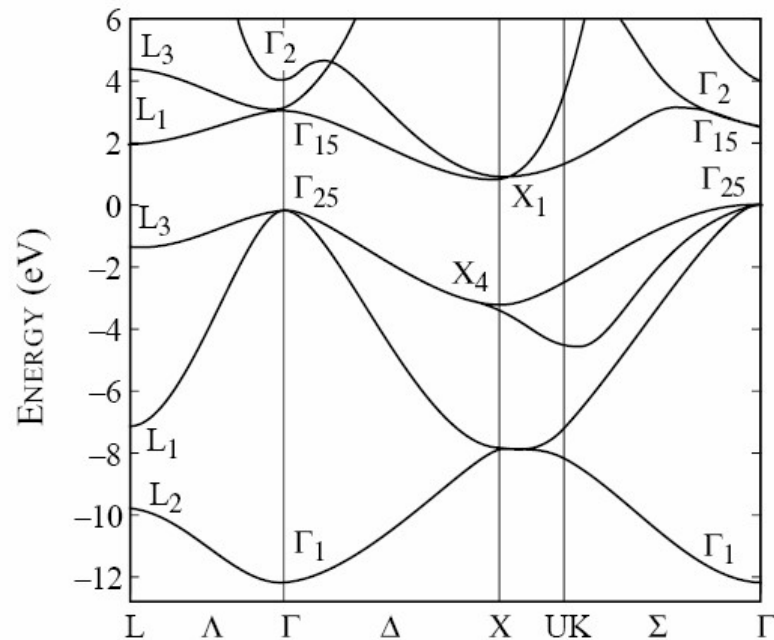
$$I \propto \sum_{\text{empty } \vec{k}} e\vec{v}_{\vec{k}}$$

# valence band, holes

---

In the valence band, the effective mass is negative.

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



# Holes

---

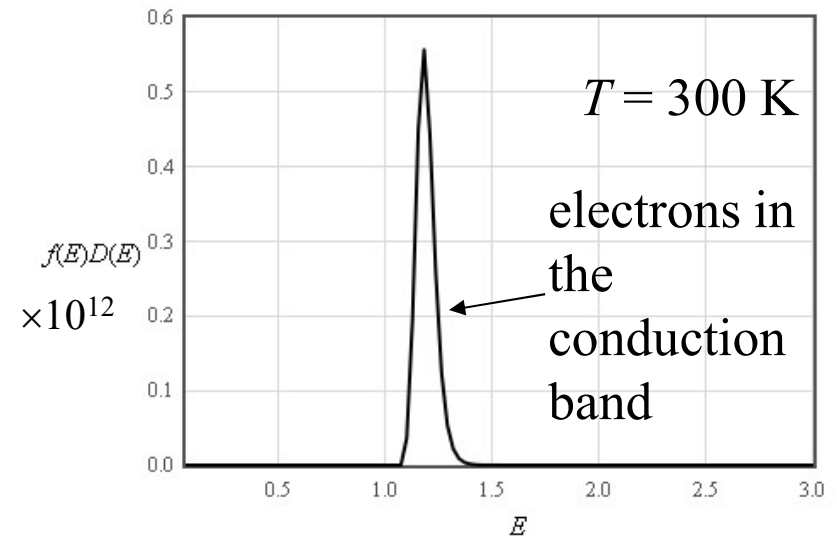
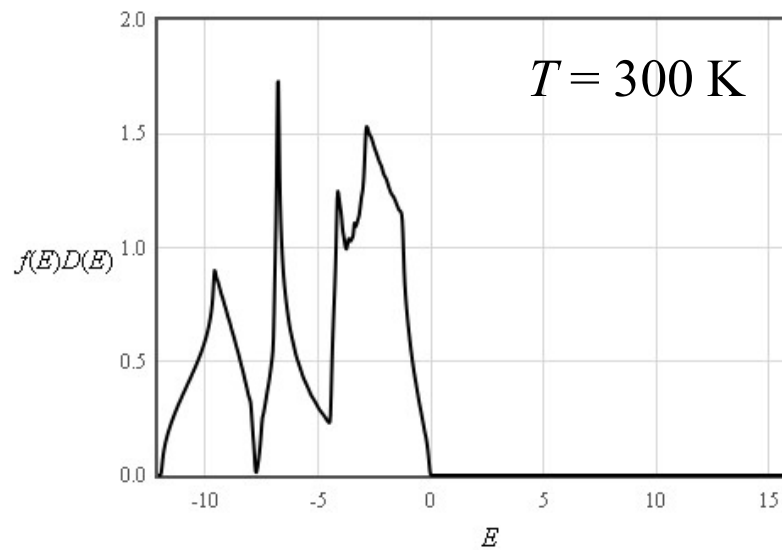
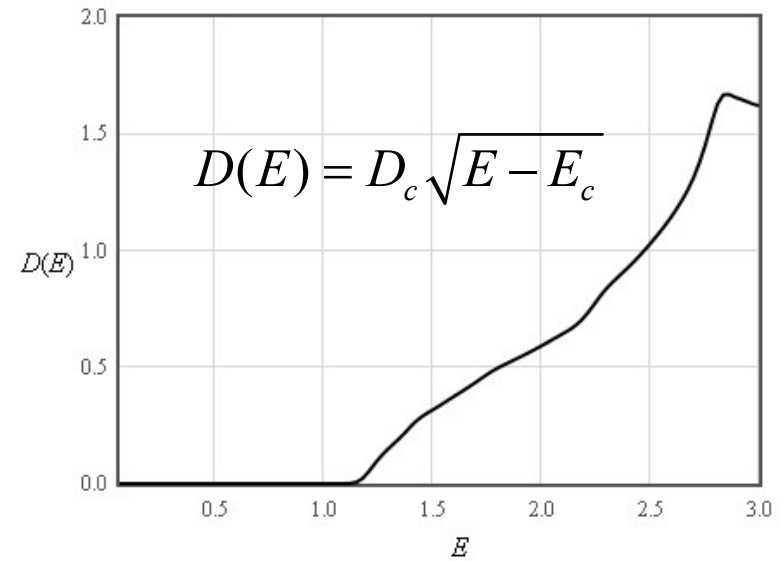
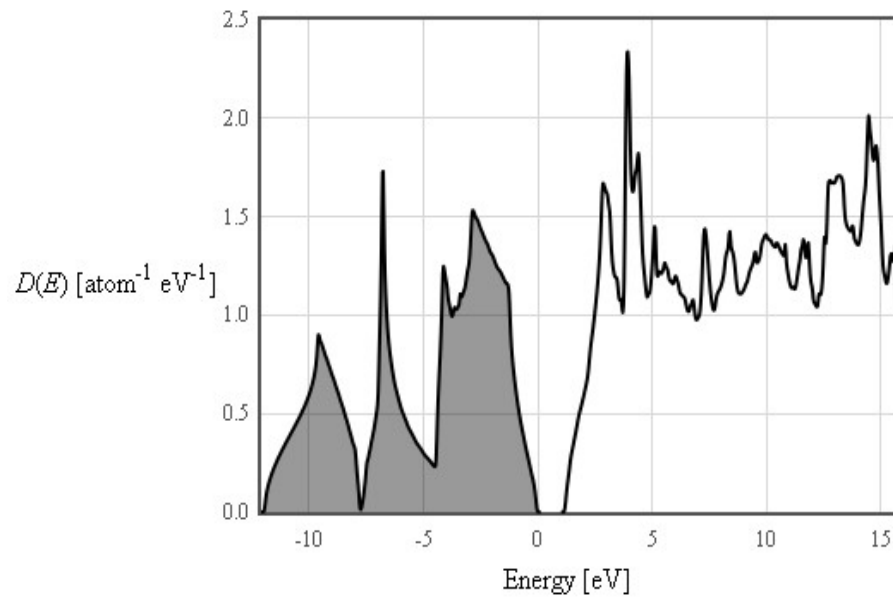
Charge carriers in the valence band can be considered to be positively charged holes. The number of holes in the valence band is the number of missing electrons.

$m_h^*$  = effective mass of holes

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

$$\vec{F} = e\vec{E} = m_h^* \vec{a}$$

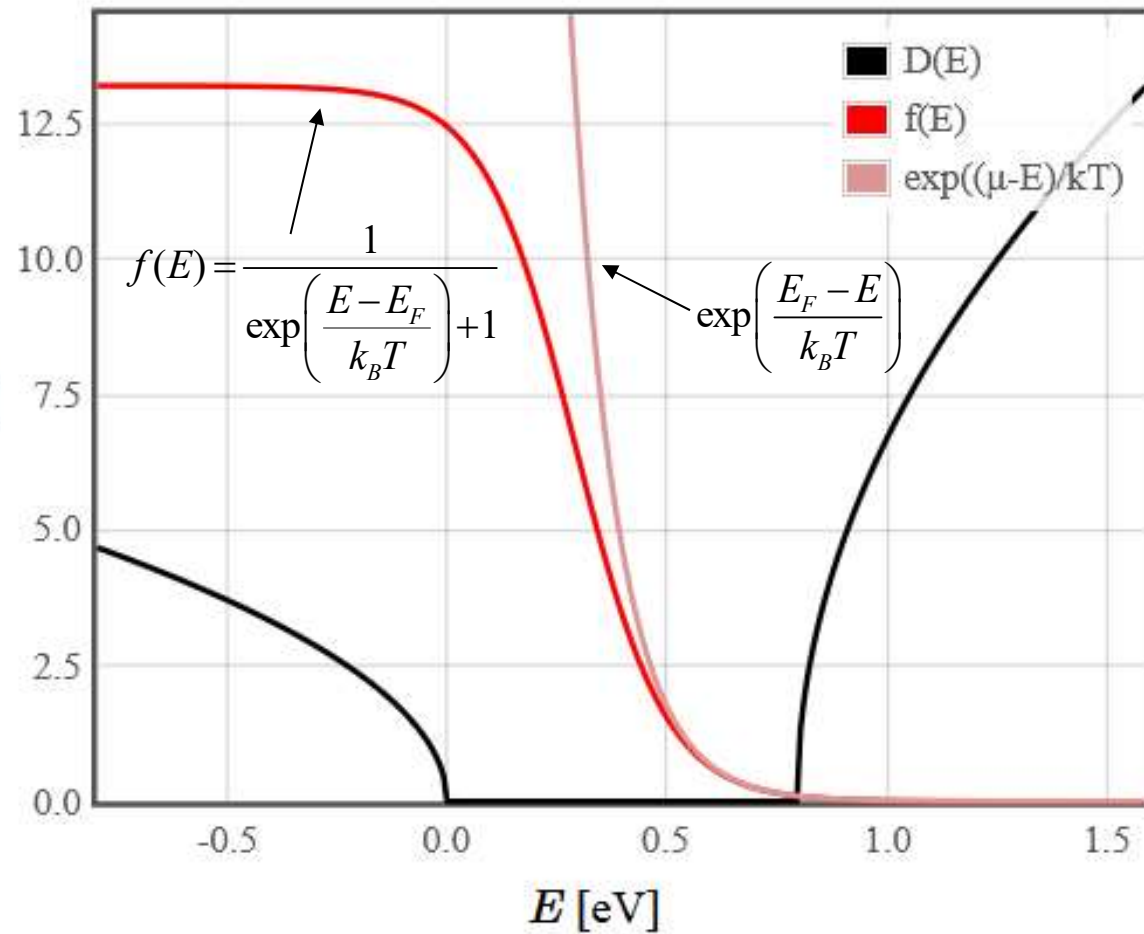
# Silicon density of states



# Boltzmann approximation

$$n = \int_{E_c}^{\infty} D(E) f(E) dE$$

$D(E)$  [eV<sup>-1</sup> cm<sup>-3</sup>]  
× 10<sup>-30</sup>





# Density of electrons in the conduction band

---

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

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

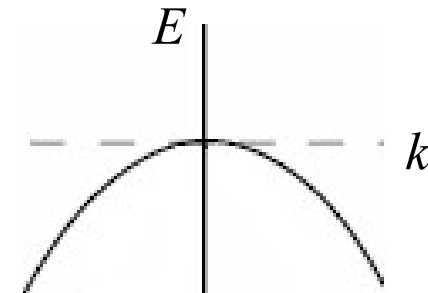
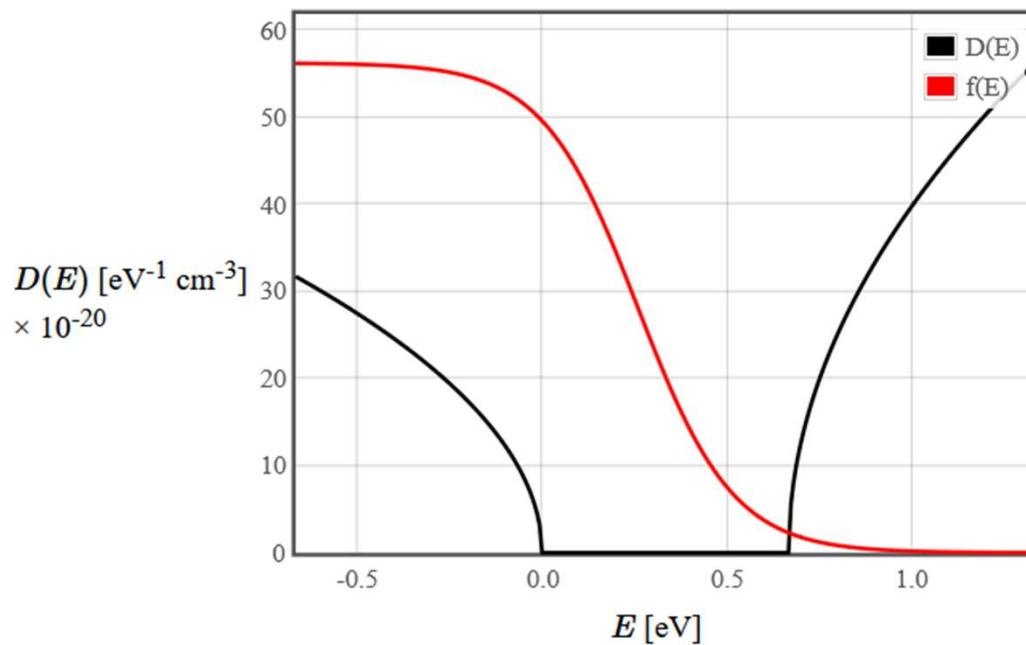
$$n = \frac{2D_c}{\sqrt{\pi}} (k_B T)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right) = \boxed{N_c(T) \exp\left(\frac{E_F - E_c}{k_B T}\right)}$$

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

# Density of holes in the valence band

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

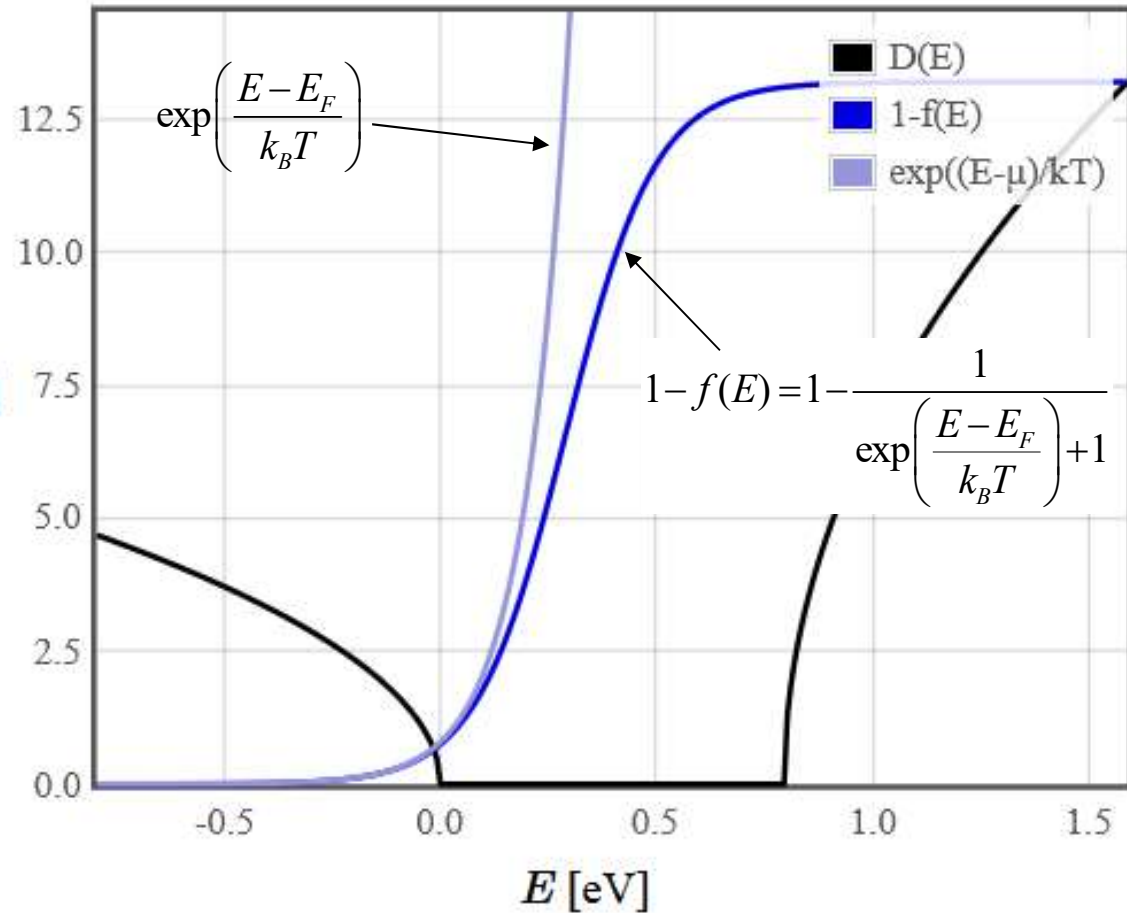
$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(\frac{E - E_F}{k_B T}\right)$$



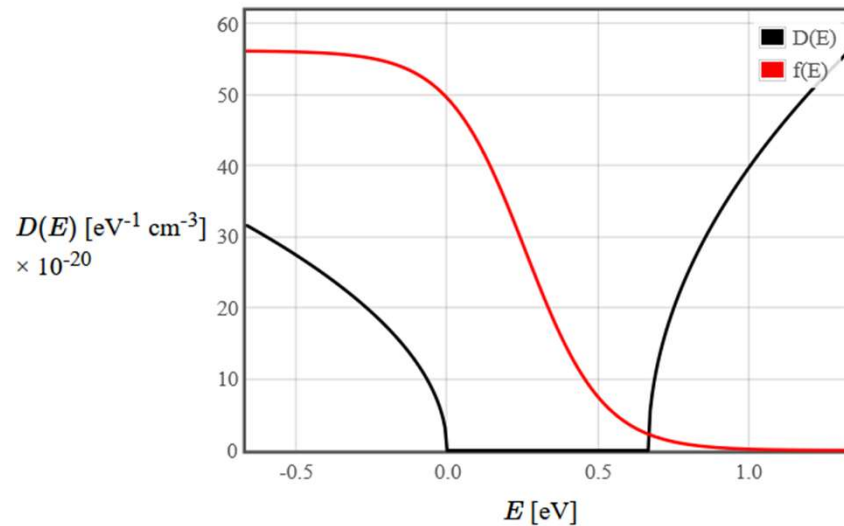
# Boltzmann approximation

$$p = \int_{-\infty}^{E_v} D(E)(1-f(E))dE$$

$D(E)$  [eV<sup>-1</sup> cm<sup>-3</sup>]  
× 10<sup>-30</sup>



# Density of holes in the valence band



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

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

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

## Boltzmann approximation

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

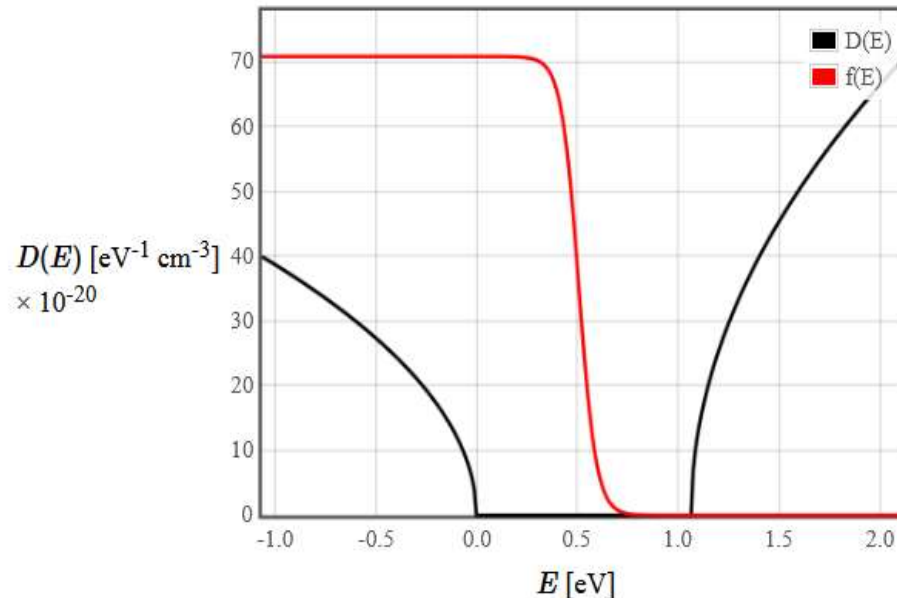
$$D(E) = \begin{cases} D_v \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

Where  $D_v$  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 'density states effective 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,

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

Data for different semiconducting materials can be found in the [NSM Archive](#).

The plot below 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 Fermi function is 1 and those states are occupied. At high energies the Fermi function goes to zero and those states are unoccupied. In the limit of low temperature, the Fermi energy is in the middle of the band gap,  $E_F = E_g/2$ . As the temperature increases, the Fermi energy moves towards the band with the lower density of states.

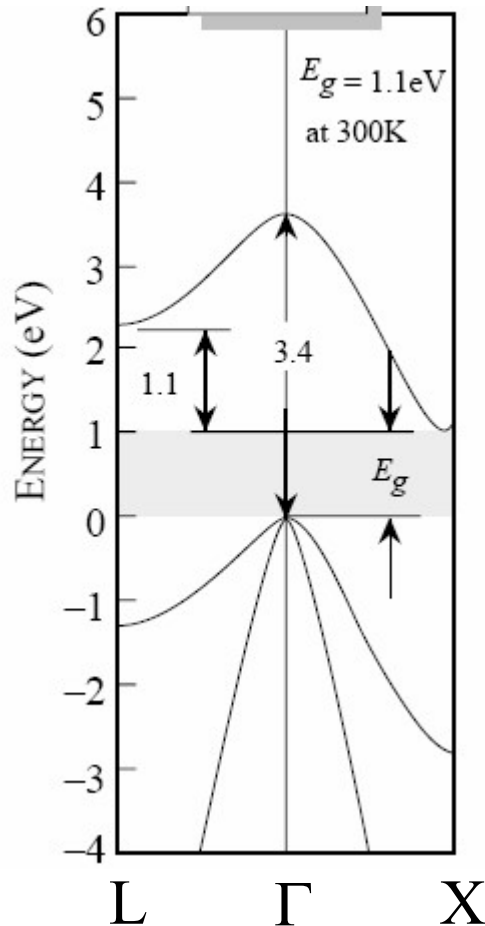


$D_c =$ <input type="text" value="6.874E21"/>	$\text{eV}^{-3/2} \text{cm}^{-3}$	Semiconductor <input type="button" value="Si"/> <input type="button" value="Ge"/> <input type="button" value="GaAs"/> <input type="button" value="GaP"/> <input type="button" value="InAs"/> <input type="button" value="InP"/> <input type="button" value="InSb"/>
$D_v =$ <input type="text" value="3.8775E21"/>	$\text{eV}^{-3/2} \text{cm}^{-3}$	
$E_g =$ <input type="text" value="1.166-4.73E-4*T*(T+636)"/>	eV	
$T =$ <input type="text" value="500"/>	K	
<input type="button" value="Replot"/>		

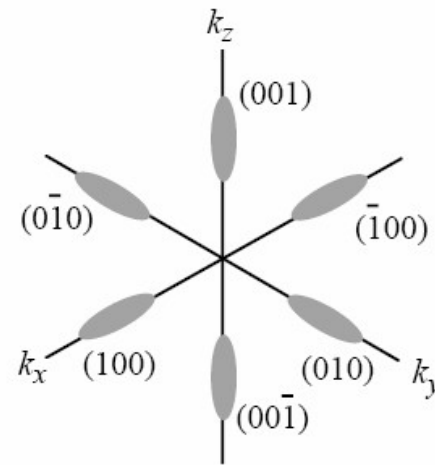
$$E_v = 0, \quad E_c = E_g = 1.062 \text{ eV}, \quad \mu = 0.5063 \text{ eV}$$

$$N_c(300) = 3.224\text{e}+19 \text{ cm}^{-3}, \quad N_v(300) = 1.819\text{e}+19 \text{ cm}^{-3}$$

# Density of electrons in the conduction band



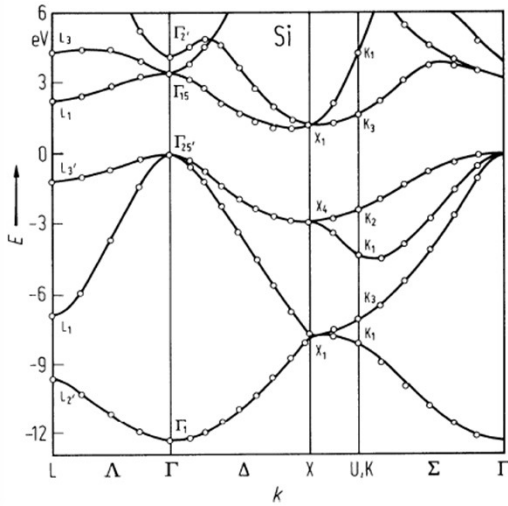
$$n = 2 \left( \frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} \exp \left( \frac{E_F - E_c}{k_B T} \right)$$



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

Properties	Si	Ge	GaAs
Bandgap $E_g$	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) $N_c$	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$

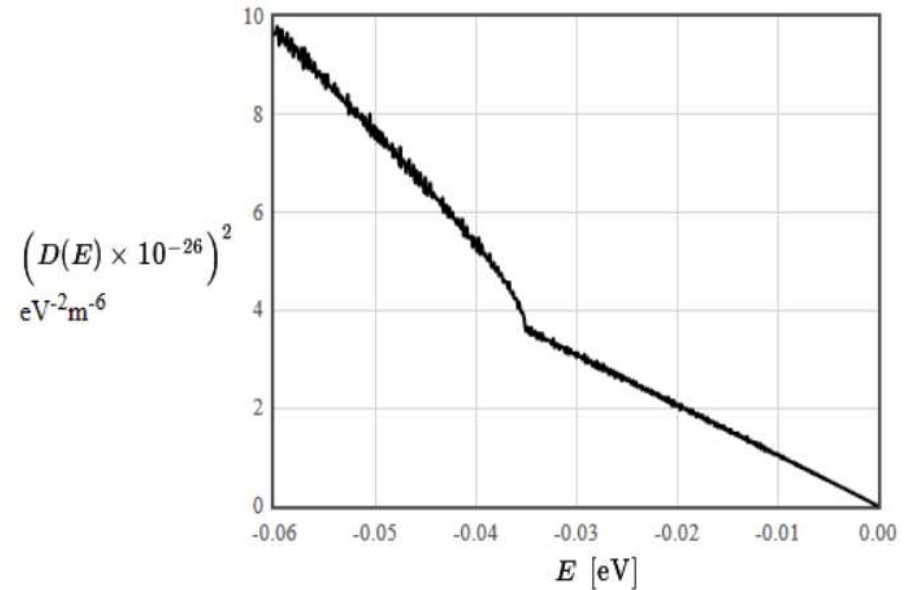
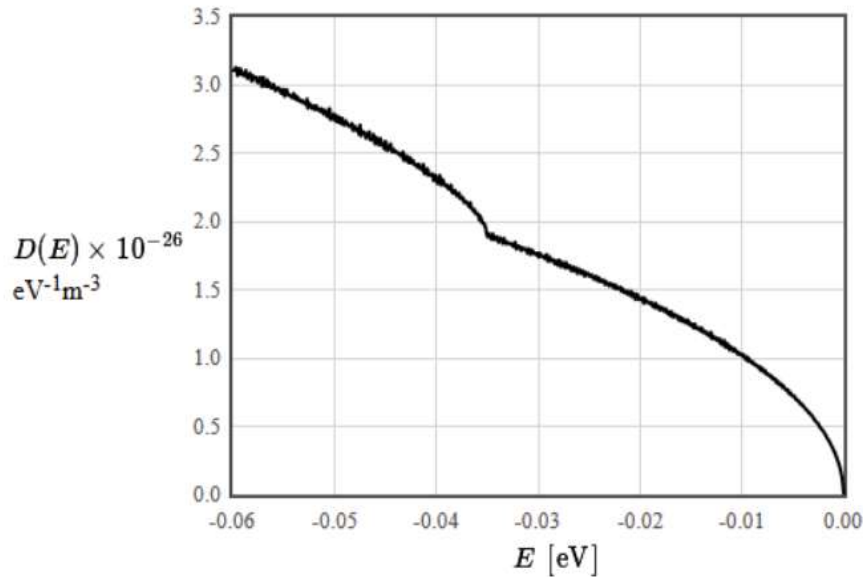
# Silicon valence bands



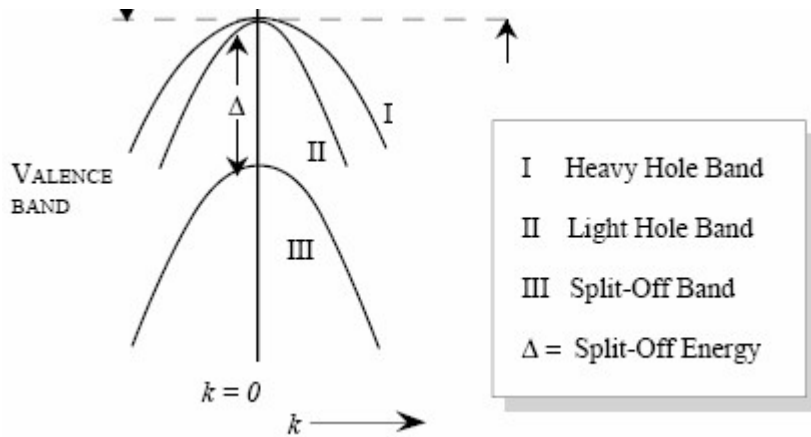
$$E_{v,th} = -\frac{\hbar^2}{2m_e} \left( 4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right),$$

$$E_{v,hh} = -\frac{\hbar^2}{2m_e} \left( 4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right),$$

$$E_{v,so} = -E_{so} - \frac{\hbar^2k^2}{2m_{so}}.$$



# Density of holes in the valence band



$$p = 2 \left( \frac{m_h^* k_B T}{2\pi\hbar^2} \right)^{3/2} \exp\left( \frac{E_v - E_F}{k_B T} \right)$$

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

Properties	Si	Ge	GaAs
Bandgap $E_g$	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) $N_c$	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
Effective density of states in valence band (300 K) $N_v$	$9.84 \times 10^{24} \text{ m}^{-3}$	$6.0 \times 10^{24} \text{ m}^{-3}$	$7.72 \times 10^{24} \text{ m}^{-3}$
Effective mass electrons $m^*/m_0$	$m_l^* = 0.98$ $m_t^* = 0.19$	$m_l^* = 1.64$ $m_t^* = 0.082$	$m^* = 0.067$
Effective mass holes $m^*/m_0$	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$
Crystal structure	diamond	diamond	zincblende
Density	2.328 g/cm <sup>3</sup>	5.3267 g/cm <sup>3</sup>	5.32 g/cm <sup>3</sup>
Atoms/m <sup>3</sup>	$5.0 \times 10^{28}$	$4.42 \times 10^{28}$	$4.42 \times 10^{28}$



# New Semiconductor Materials. Biology systems. Characteristics and Properties

Semiconductors database	n,k InGaAsP	Levels	Equivalents	Bibliografic database
----------------------------	----------------	--------	-------------	-----------------------

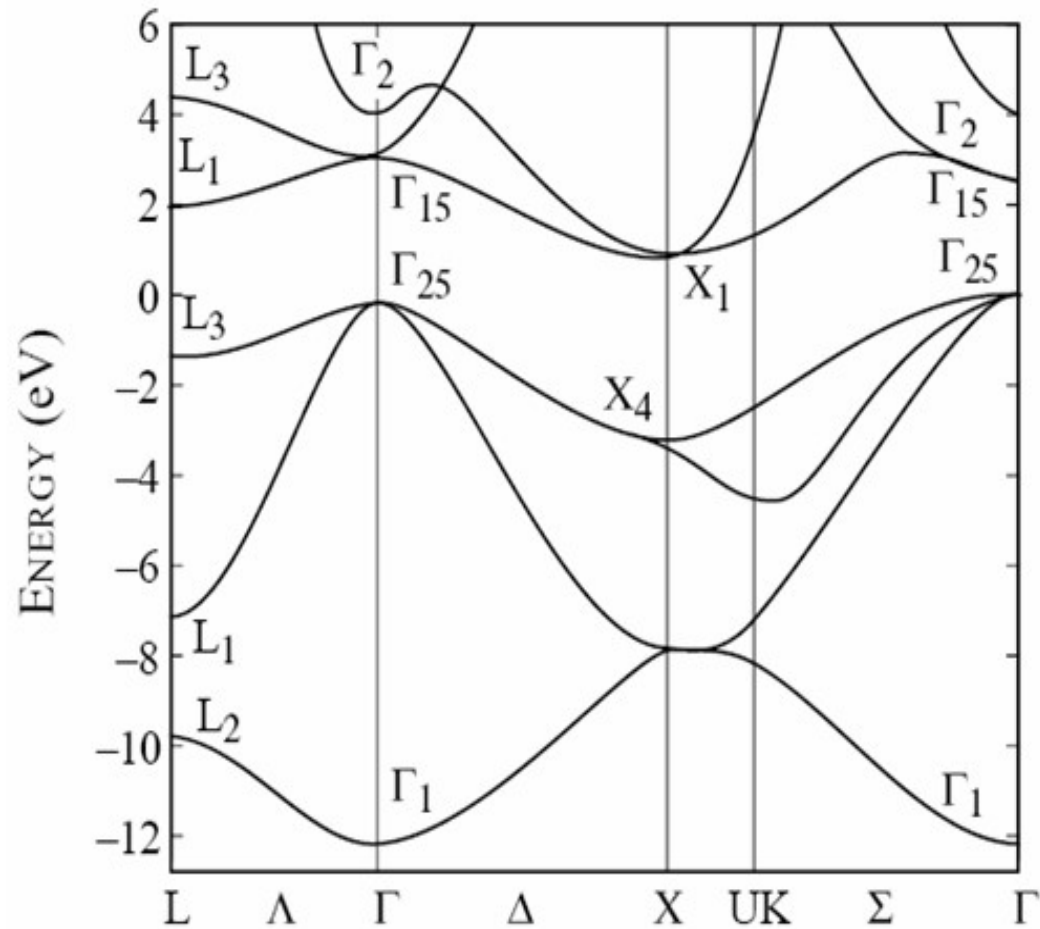
## NSM Archive - Physical Properties of Semiconductors

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 <sub>1-x</sub> Sb <sub>x</sub>	- Gallium Arsenide Antimonide
Al <sub>x</sub> Ga <sub>1-x</sub> As	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride	InN	- Indium Nitride
BN	- Boron Nitride	GaN	- Gallium Nitride

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

## Exam March 2007 Problem 1

The band structure of a semiconductor is shown below. The zero of energy is chosen to be the top of the valence band.



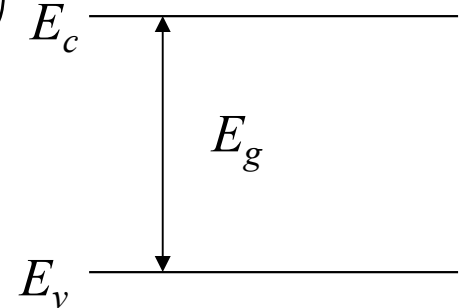
- Is this a direct or an indirect semiconductor? Why?
- What is the band gap?
- What are light holes and heavy holes? Explain how you can determine the effective mass of the holes from this diagram.

# Law of mass action

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

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



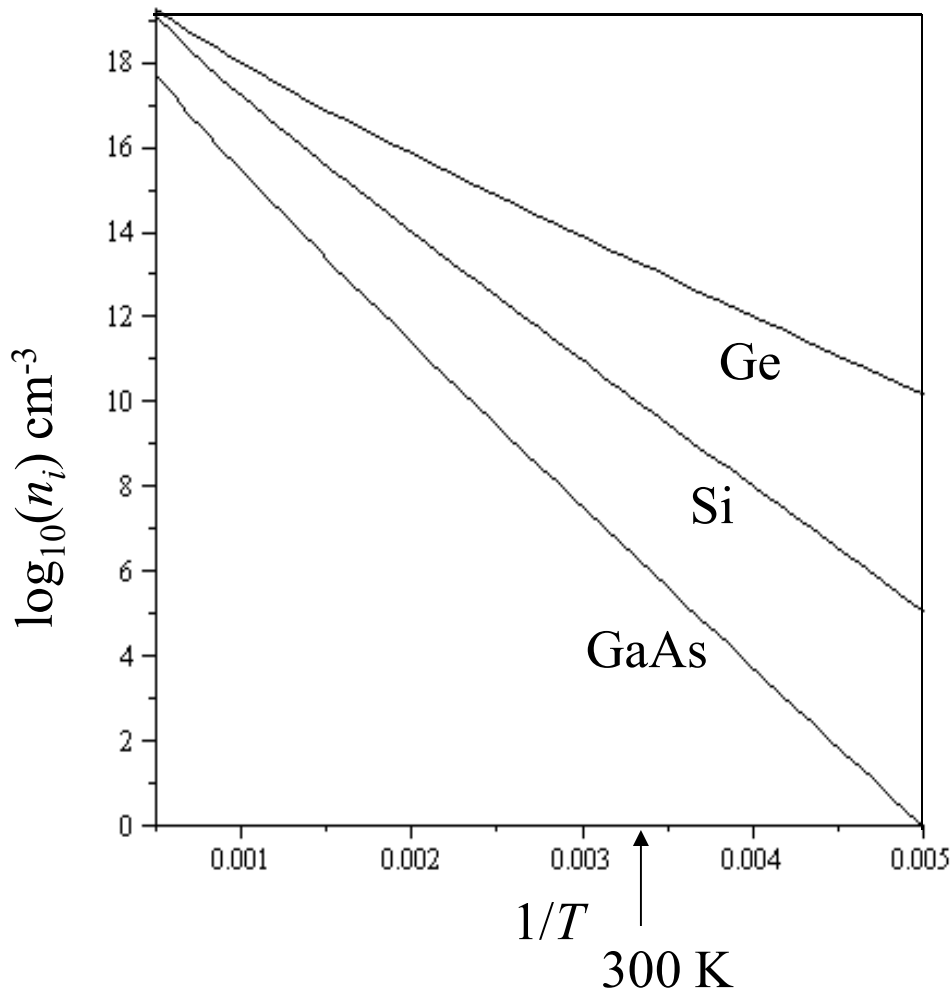
For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

# Intrinsic carrier concentration

---



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

Silicon has  $\sim 5 \times 10^{22}$  atoms/cm<sup>3</sup>

Good for thermometer, bad for designing circuits.

# Fermi energy of an intrinsic semiconductor

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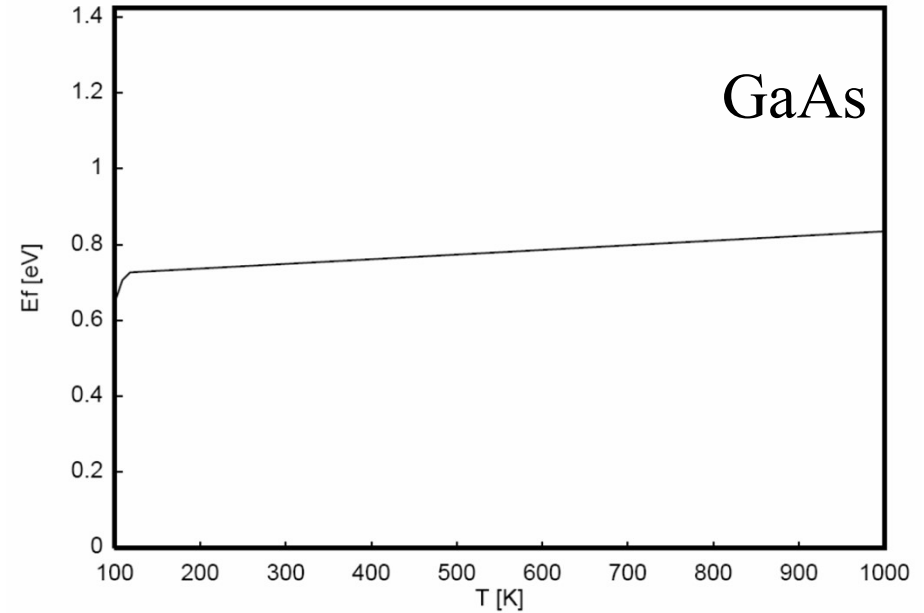
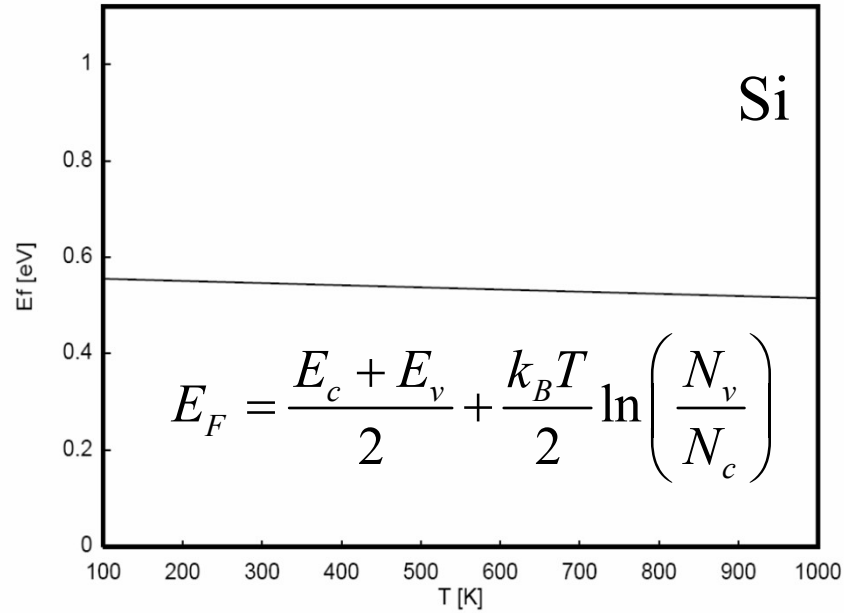
$$n = p = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

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

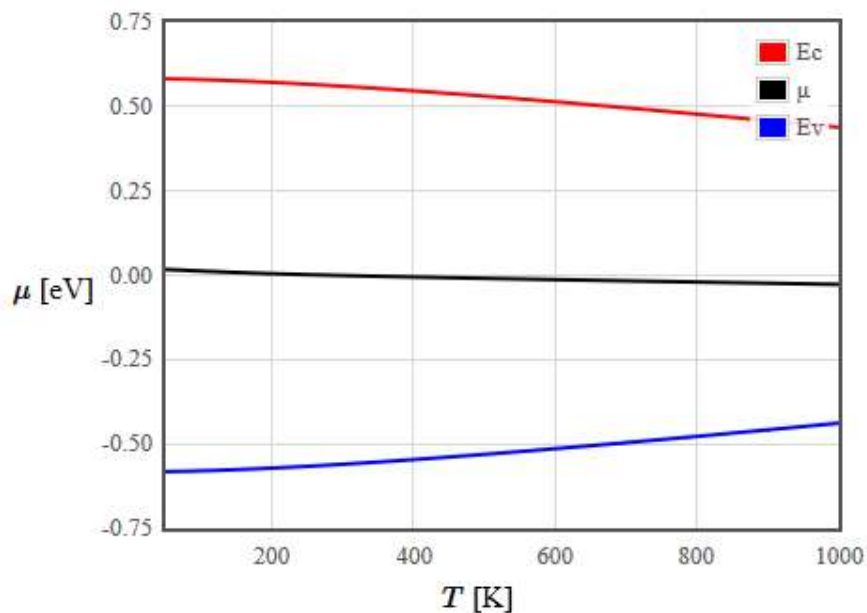
$$E_F = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)$$

# Temperature dependence of $E_F$



Properties	Si	Ge	GaAs
Bandgap $E_g$	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) $N_c$	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
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# Intrinsic semiconductors



$N_c(300\text{ K}) =$	<input type="text" value="2.78E19"/>	1/cm <sup>3</sup>
$N_v(300\text{ K}) =$	<input type="text" value="9.84E18"/>	1/cm <sup>3</sup>
$N_{so}(300\text{ K}) =$	<input type="text" value="2.98E18"/>	1/cm <sup>3</sup>
$E_g =$	<input type="text" value="1.166-4.73E-4*T*T/(T+636)"/>	eV
$E_v - E_{so} =$	<input type="text" value="0.044"/>	eV
$T_1 =$	<input type="text" value="50"/>	K
$T_2 =$	<input type="text" value="1000"/>	K
<input type="button" value="Replot"/>		

Semiconductor

[http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic\\_so.php](http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic_so.php)

# Extrinsic semiconductors

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The introduction of impurity atoms that can add electrons or holes is called doping.

n-type : donor atoms contribute electrons to the conduction band.  
Examples: P, As in Si.

p-type : acceptor atoms contribute holes to the valence band.  
Examples: B, Ga, Al in Si.



# n and p

---

The electron density and hole density are:

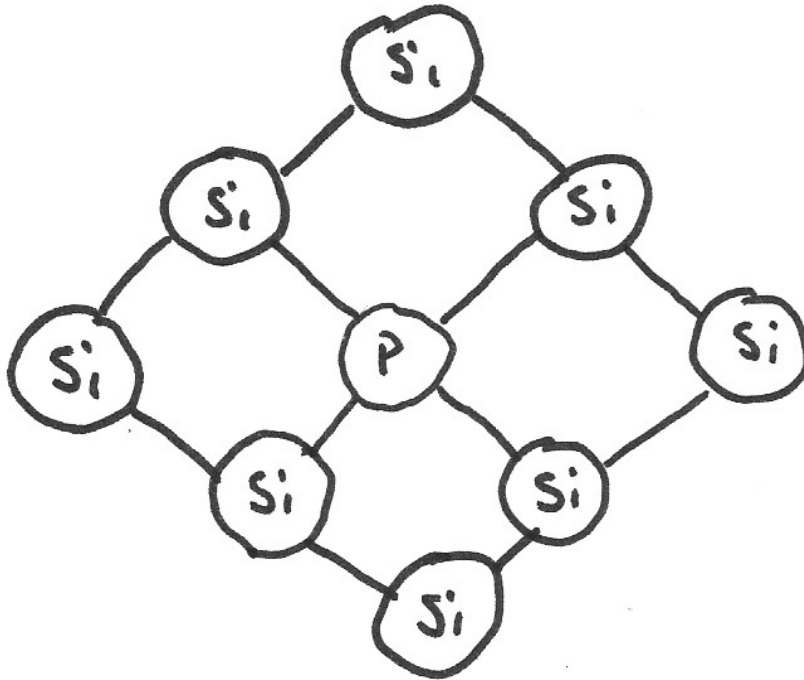
$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) \quad p = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

The law of mass action:

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

# Ionization of dopants

---



Easier to ionize a P atom in Si than a free P atom

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2 n^2}$$

Ionization energy is smaller by a factor:

$$\frac{m^*}{m} \left( \frac{\epsilon_0}{\epsilon_r \epsilon_0} \right)^2$$

Ionization energy  $\sim 25$  meV

	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
IIB	30 Zn	31 Ga	32 Ge	33 As
	34 Se			
	48 Cd	49 In	50 Sn	51 Sb
				52 Te

acceptors in Si



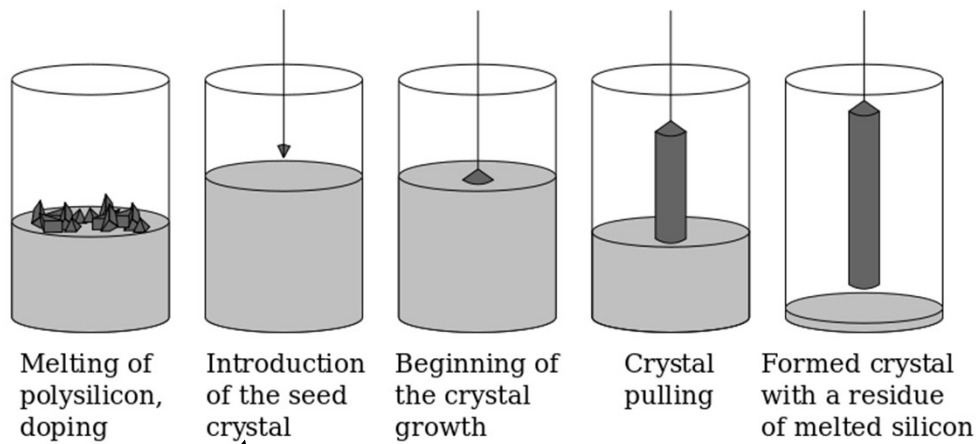
donors in Si



# Crystal growth

---

## Czochralski Process



add dopants to the melt



images from wikipedia

# Crystal growth

---

## Float zone Process

Neutron transmutation

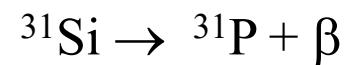
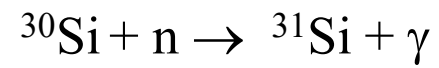


image from wikipedia

# Gas phase diffusion

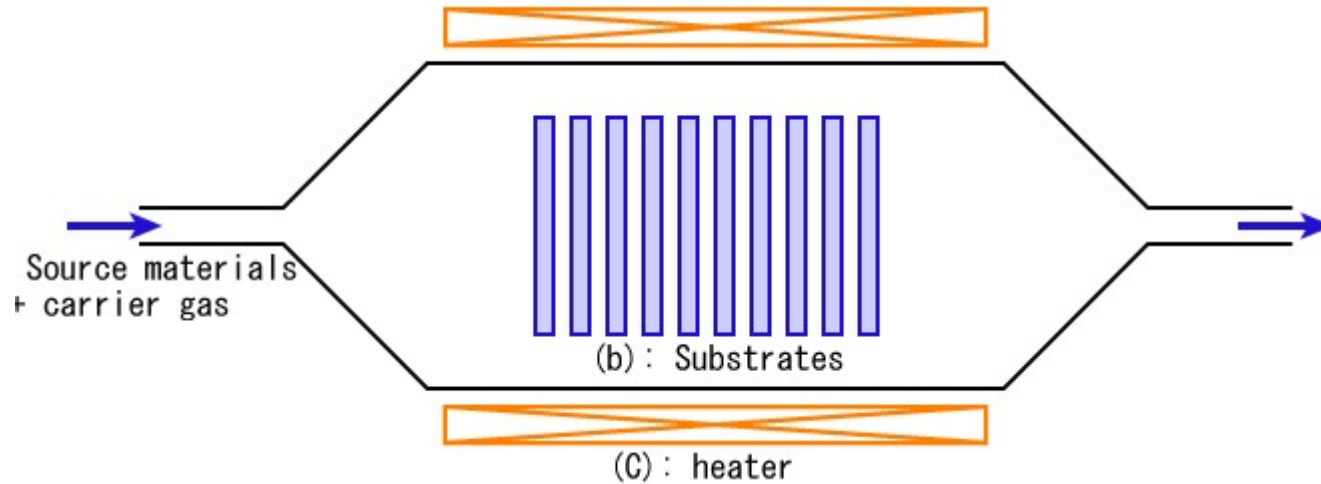
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$\text{AsH}_3$  (Arsine) or  $\text{PH}_3$  (phosphine) for n-doping  
 $\text{B}_2\text{H}_6$  (diborane) for p-doping.

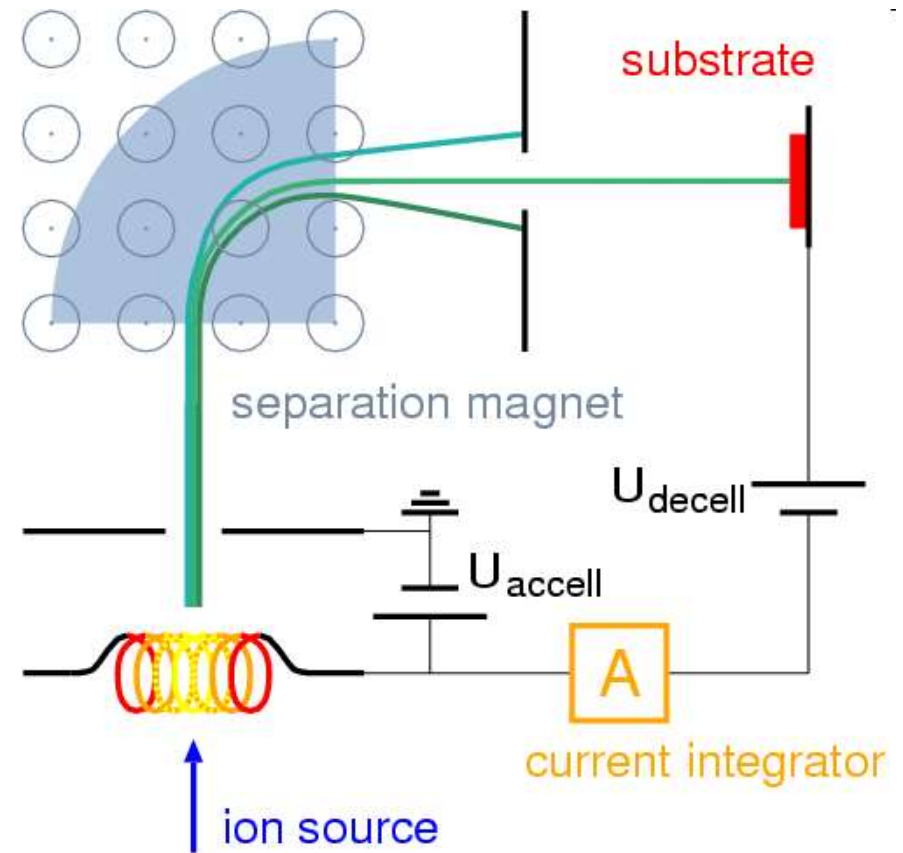
# Chemical vapor deposition

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Epitaxial silicon CVD  $\text{SiH}_4$  (silane) or  $\text{SiH}_2\text{Cl}_2$  (dichlorosilane)  
 $\text{PH}_3$  (phosphine) for n-doping or  $\text{B}_2\text{H}_6$  (diborane) for p-doping.

# Ion implantation



Implant at  $7^\circ$  to avoid channeling



# *SRIM*

## *The Stopping and Range of Ions in Matter*

*James F. Ziegler, Jochen P. Biersack, Matthias D. Ziegler*

- Ch 1 - **Historical Review**
- Ch 2 - **Nuclear Stopping of Ions**
- Ch 3 - **Electronic Stopping of Ions**
- Ch 4 - **Stopping of Energetic Light Ions**
- Ch 5 - **Stopping of Ions in Compounds**
- Ch 6 - **Ion Straggling**
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