Intrinsic semiconductors

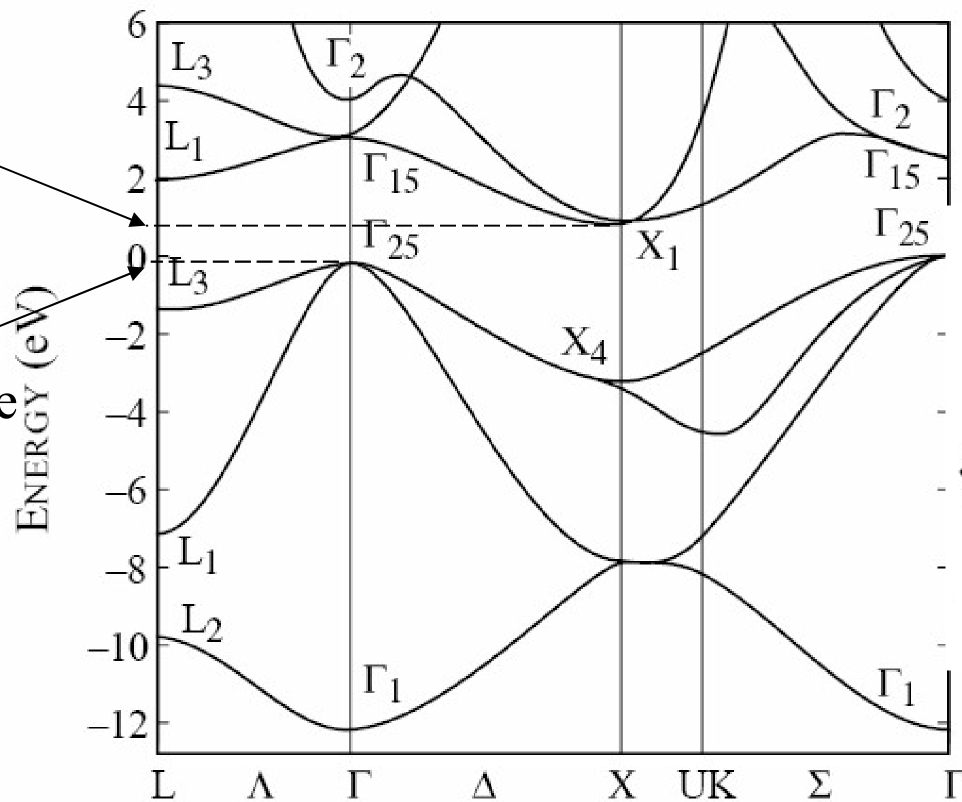
- More details of the band structure of silicon.
- Effective mass
- Electrons in the conduction band
- Holes in the valence band
- Intrinsic carrier densities

Silicon band structure

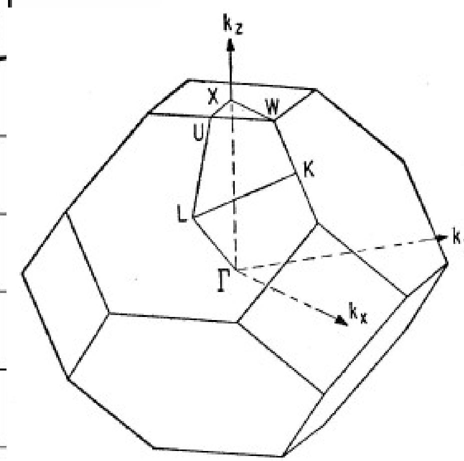
E_c = bottom of the conduction band

$$E_g = E_c - E_v$$

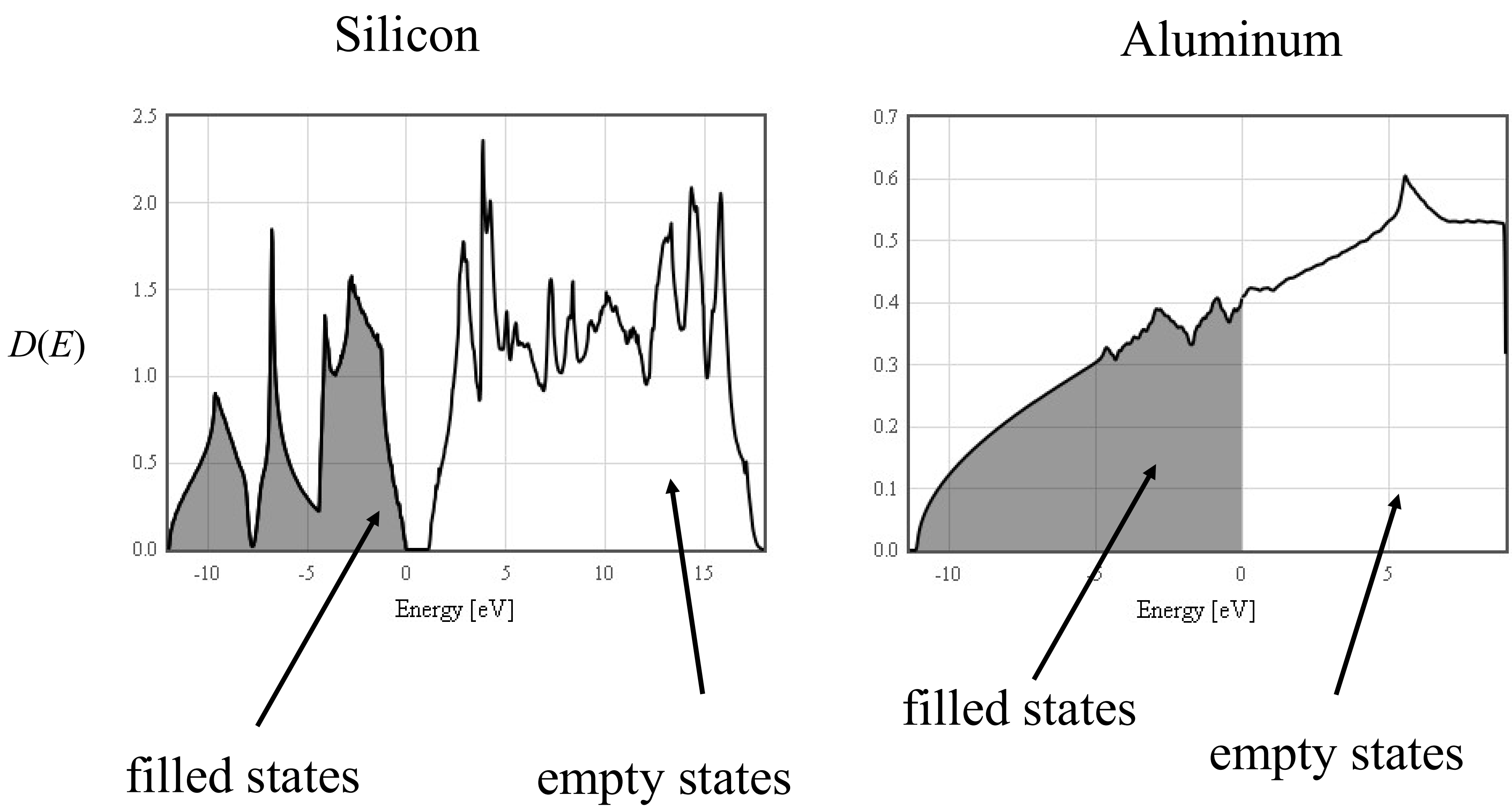
E_v = top of the valence band



[111] k=0 [100]



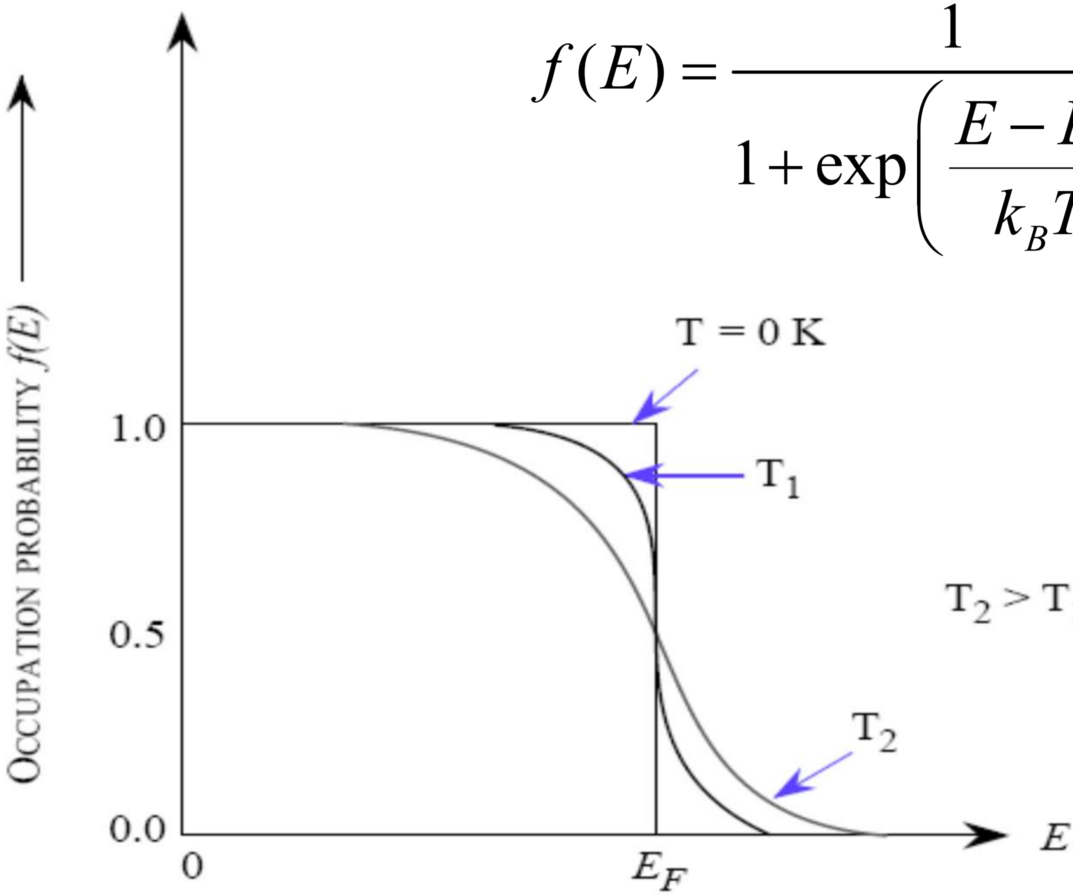
Density of states



Fermi function

f(*E*) is the probability that a state at energy *E* is occupied.

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



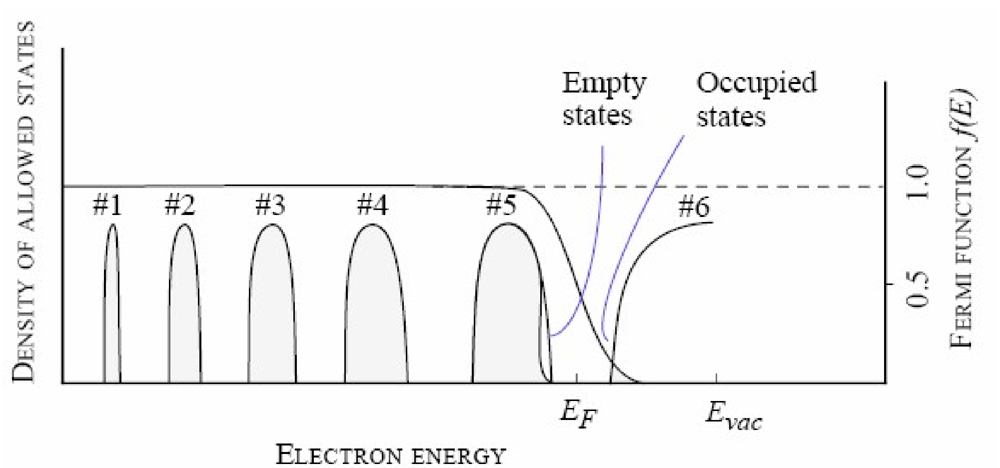
Fermi energy

The Fermi energy is implicitly defined as the energy that solves the following equation.

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

Here n is the electron density.

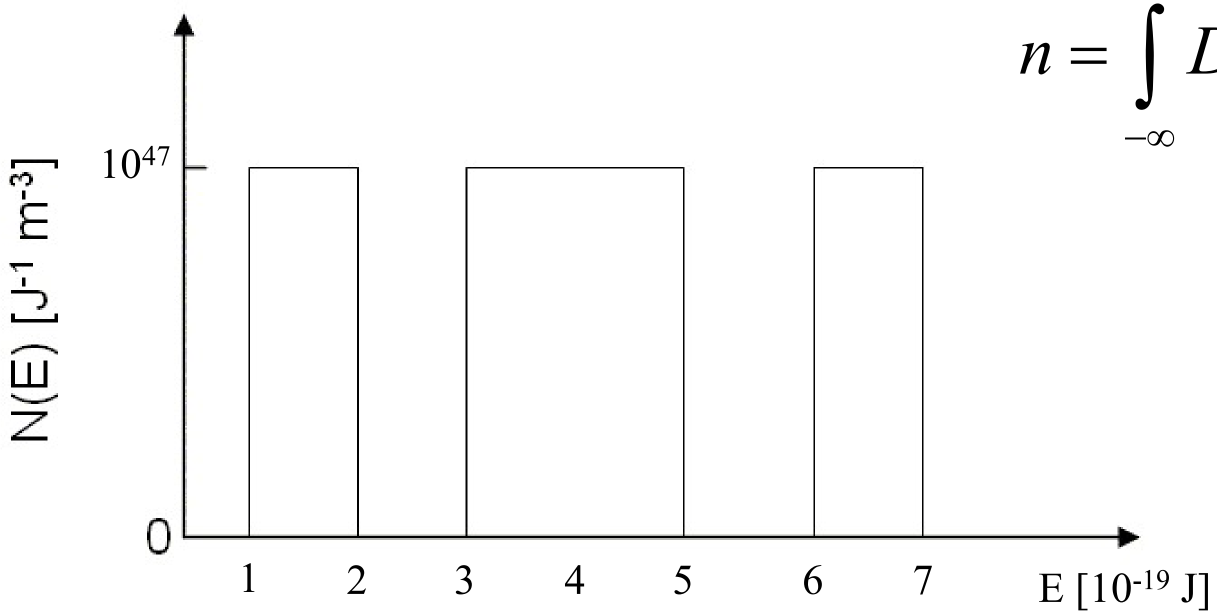
The density of states, the total number of electrons and the temperature are given. To find the Fermi energy, guess one and evaluate the integral. If n turns out too low, guess a higher E_F and if n turns out too high, guess a lower E_F.



Calculate the Fermi energy

The density of states for a particular material is given in the following figure.

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



$$n = 3\times10^{28}\ \text{m}^{-3}$$

What is the Fermi energy at zero temperature? For a semiconductor, find the limiting value of the Fermi energy as the temperature approaches zero.

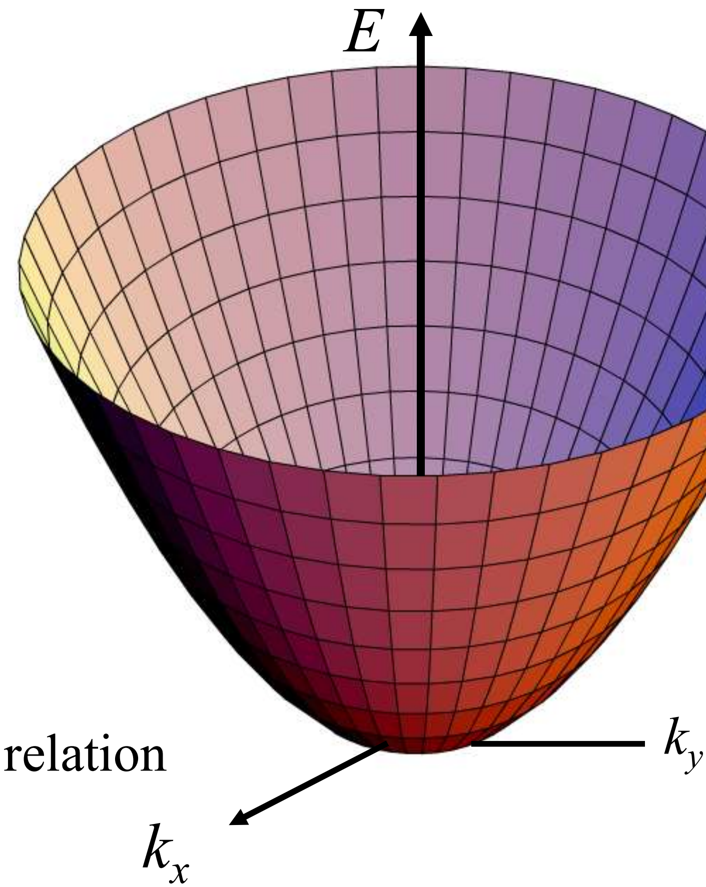
E_f = [ ] eV

What kind of material is this?

Metal

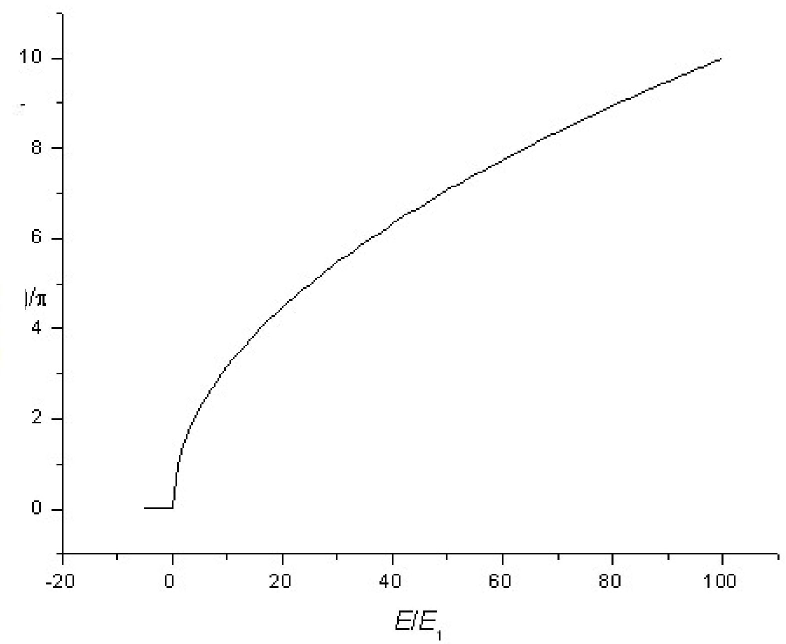
free electrons (simple model for a metal)

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



dispersion relation

3-d density of states



$$D(E) = \begin{cases} 0 & \text{for} \quad E < 0 \\ \dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} & \text{for} \quad E > 0 \end{cases}$$

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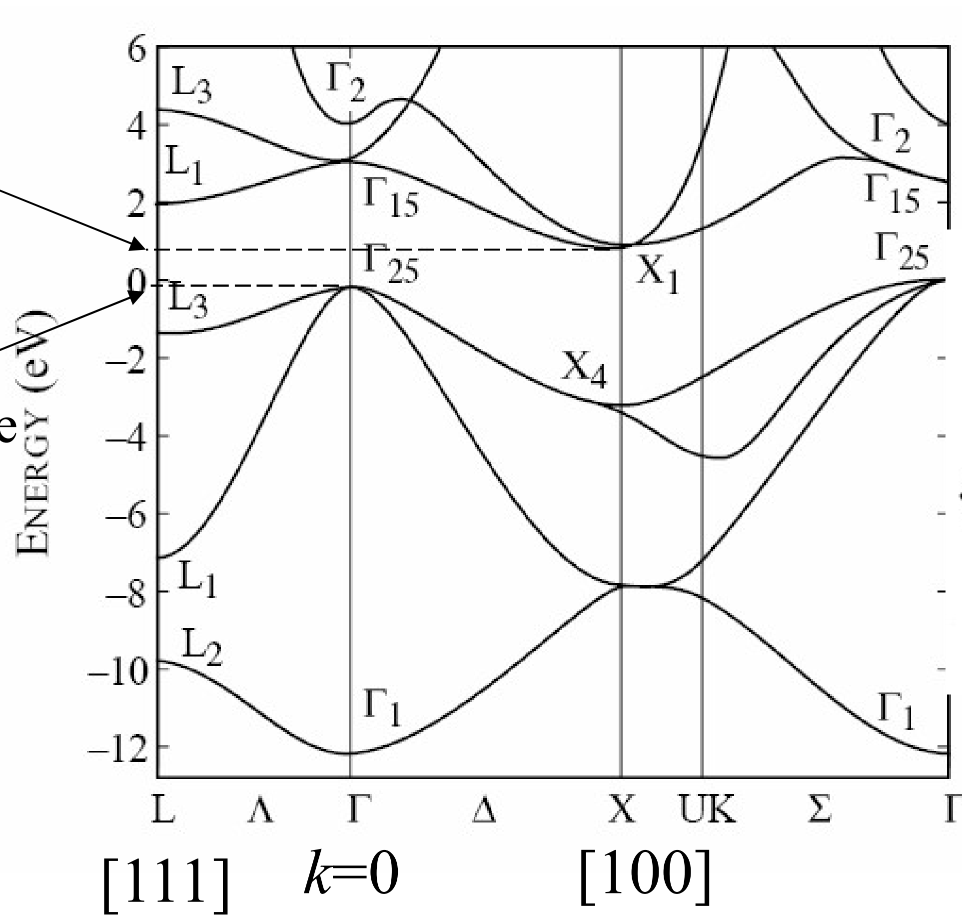
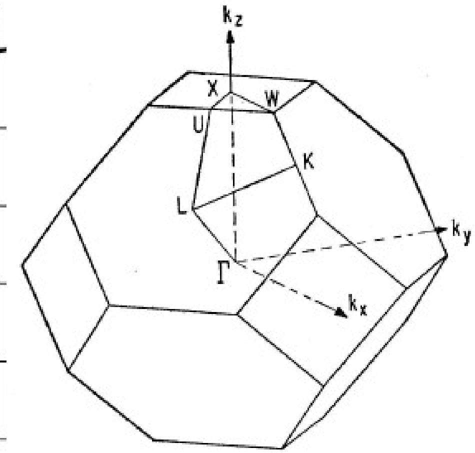
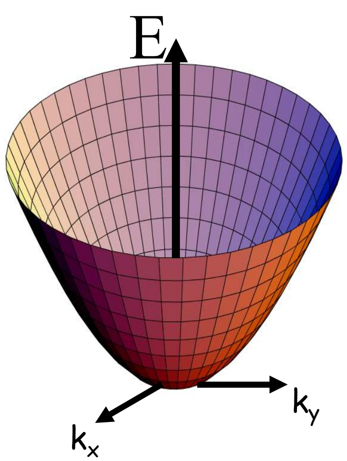






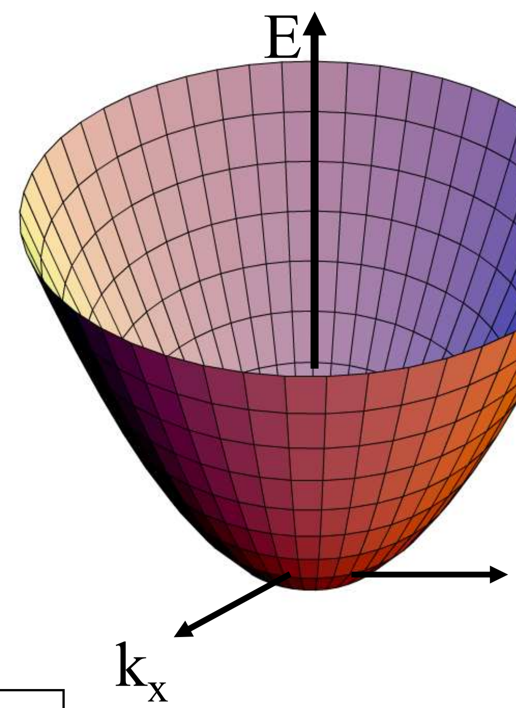
Near the bottom of the conduction band, the band structure looks like a parabola.

Effective mass

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

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

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



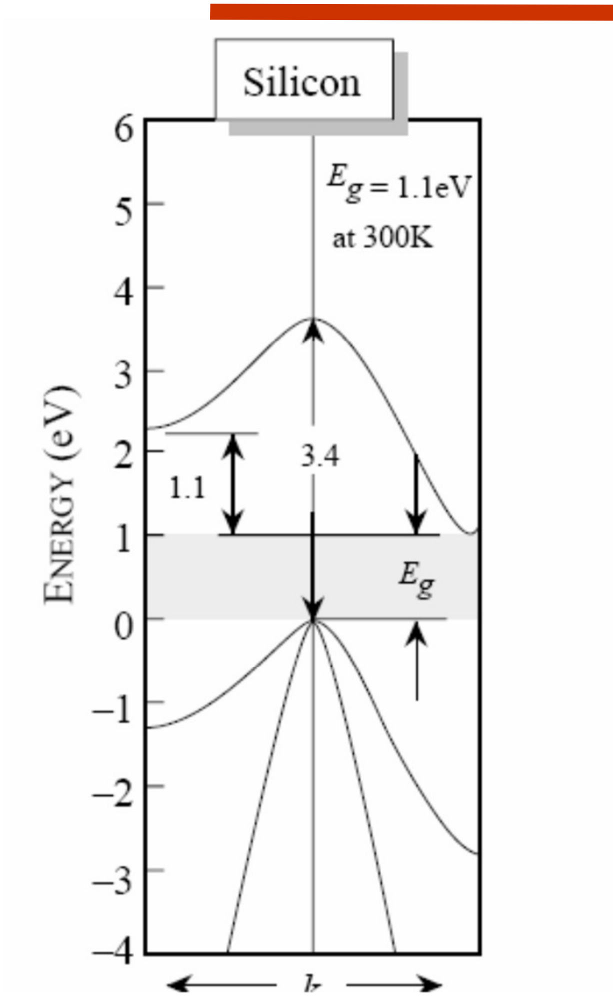
Effective mass

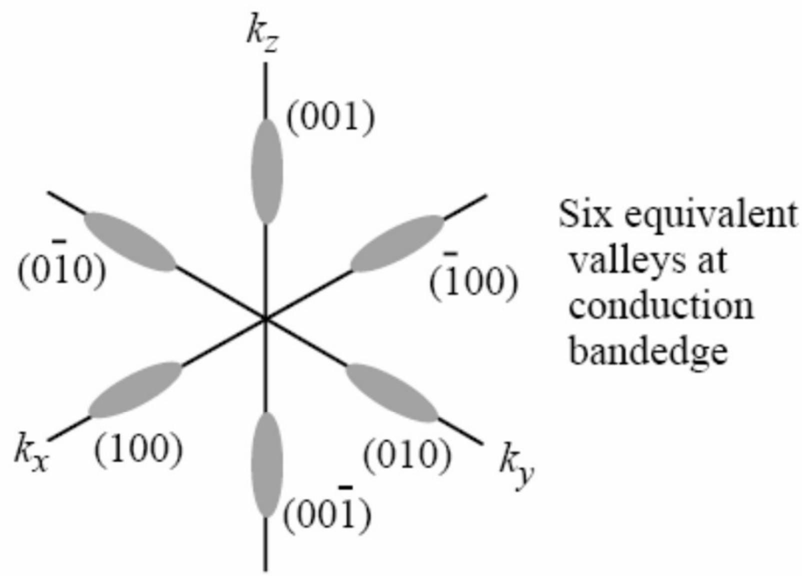
$$m_x^* = \frac{\hbar^2}{\dfrac{d^2E(\vec{k})}{dk_x^2}}$$

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

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

Anisotropic effective mass in silicon





100

The electrons seem to have different masses when the electric field is applied in different directions.

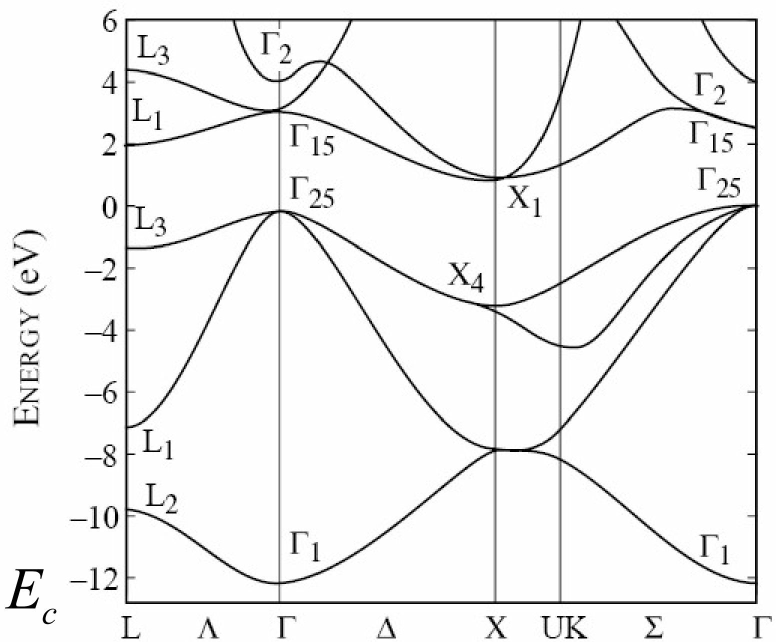
Return to problem list

Conduction band electron energy

In silicon, the bottom of the conduction valley along the (100) direction is at $(2\pi/a)(0.85,0,0)$ where $a = 0.543$ nm. Electrons in this valley have an anisotropic effective mass. The effective mass in the (100) direction is $m_l^* = 0.98m_0$ and the effective mass transverse to the [100] direction is $m_t^* = 0.19m_0$. What is the energy of an electron with a k-vector $(2\pi/a)(0.92,-0.01,0.15)$?

$E =$ [ ] eV

Submit answer | Clear



$$E = \frac{\hbar^2\left(k_x - 0.85\frac{2\pi}{a}\right)^2}{2m_l} + \frac{\hbar^2 k_y^2}{2m_t} + \frac{\hbar^2 k_z^2}{2m_t} + E_c$$

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.

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

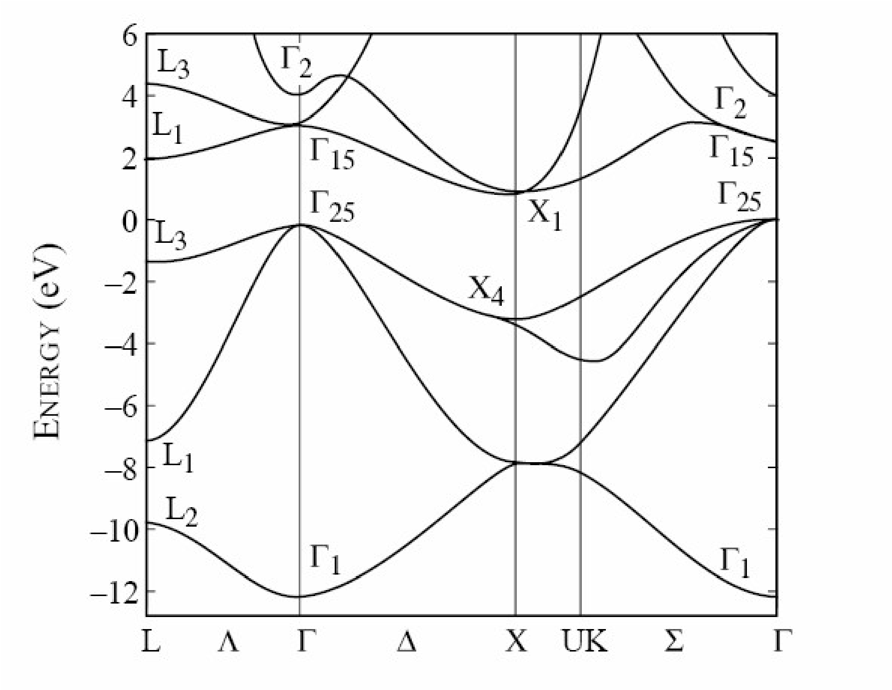
$$I \propto \sum_{\text{all } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right) - \sum_{\text{empty } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right)$$

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

valence band, holes

In the valence band, the effective mass is negative.

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



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

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

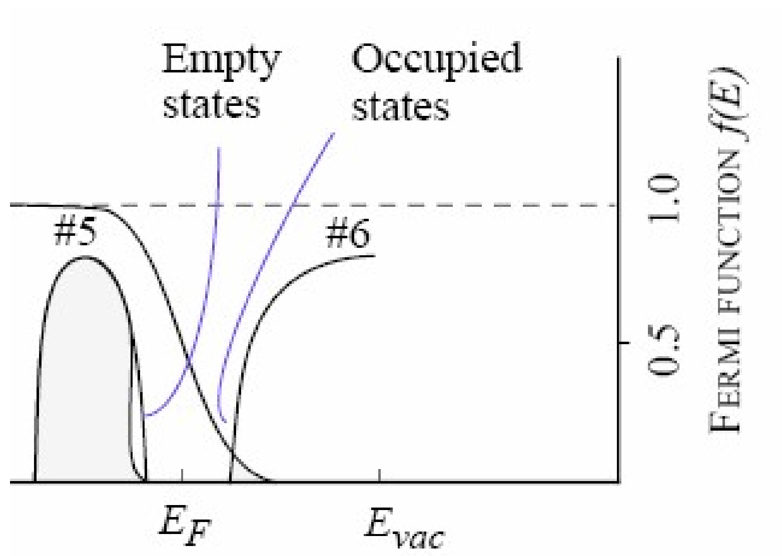
$$\vec{F} = e\vec{E} = m_h^*\vec{a}$$

Density of electrons in the conduction band

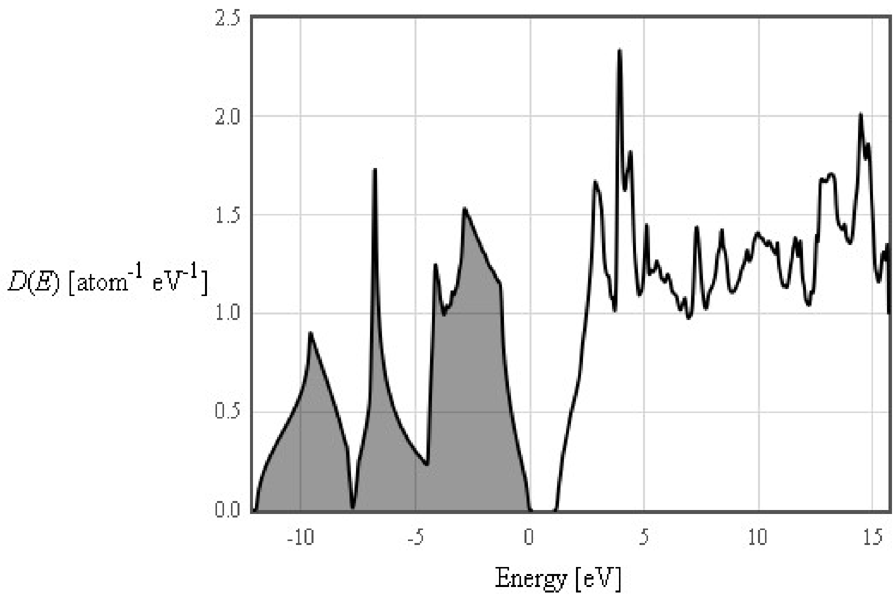
The free electron density of states is modified by the effective mass.

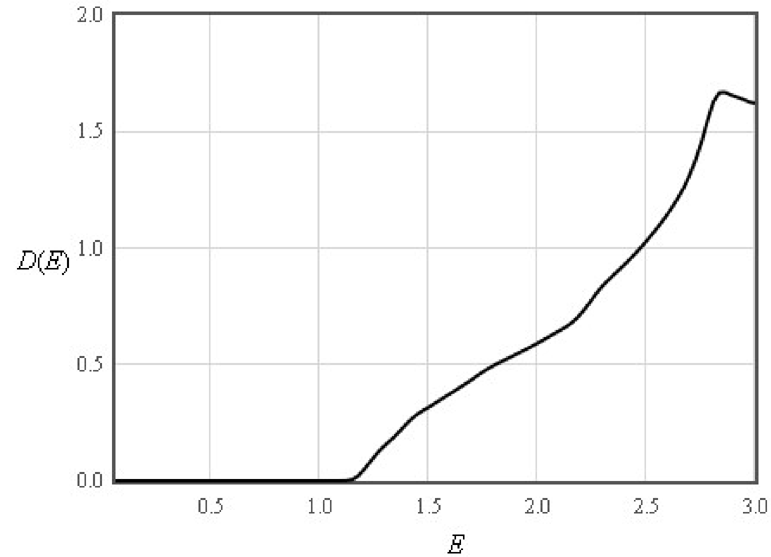
$$D(E) = \frac{\pi}{2}\left(\frac{2m^* L^2}{\hbar^2 \pi^2}\right)^{3/2}\sqrt{E - E_c}$$

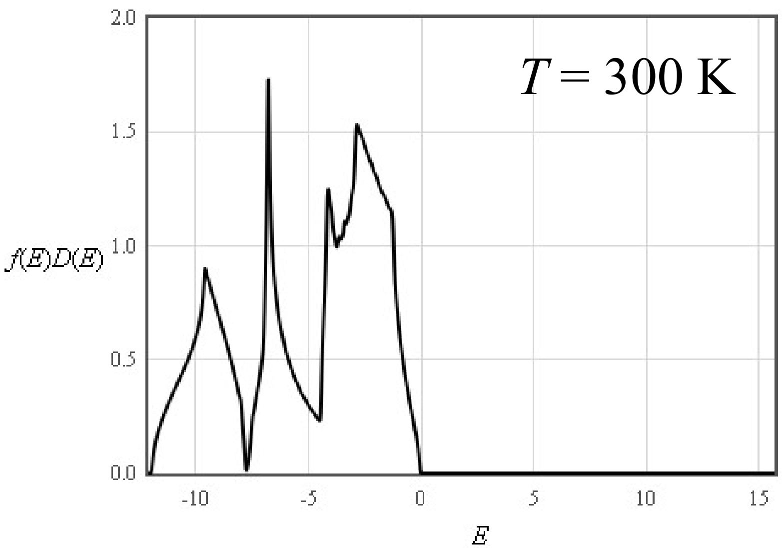
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(\frac{E_F - E}{k_B T}\right)$$

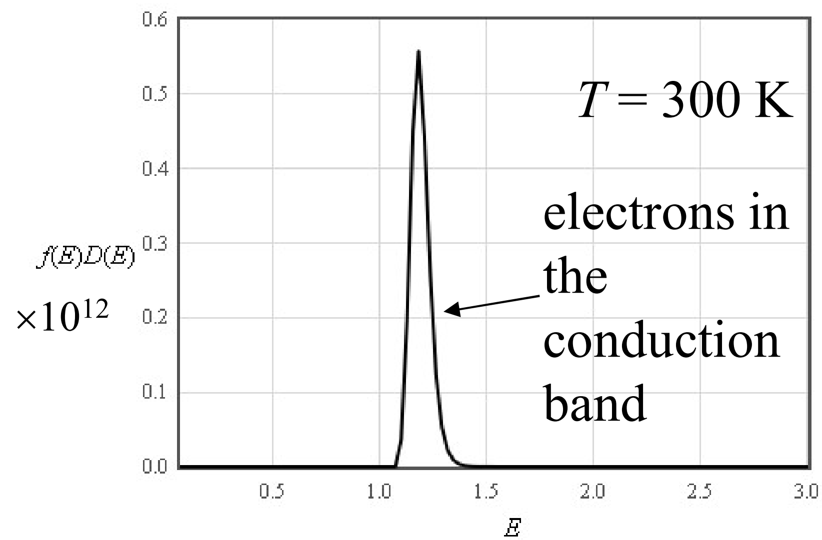


Silicon density of states

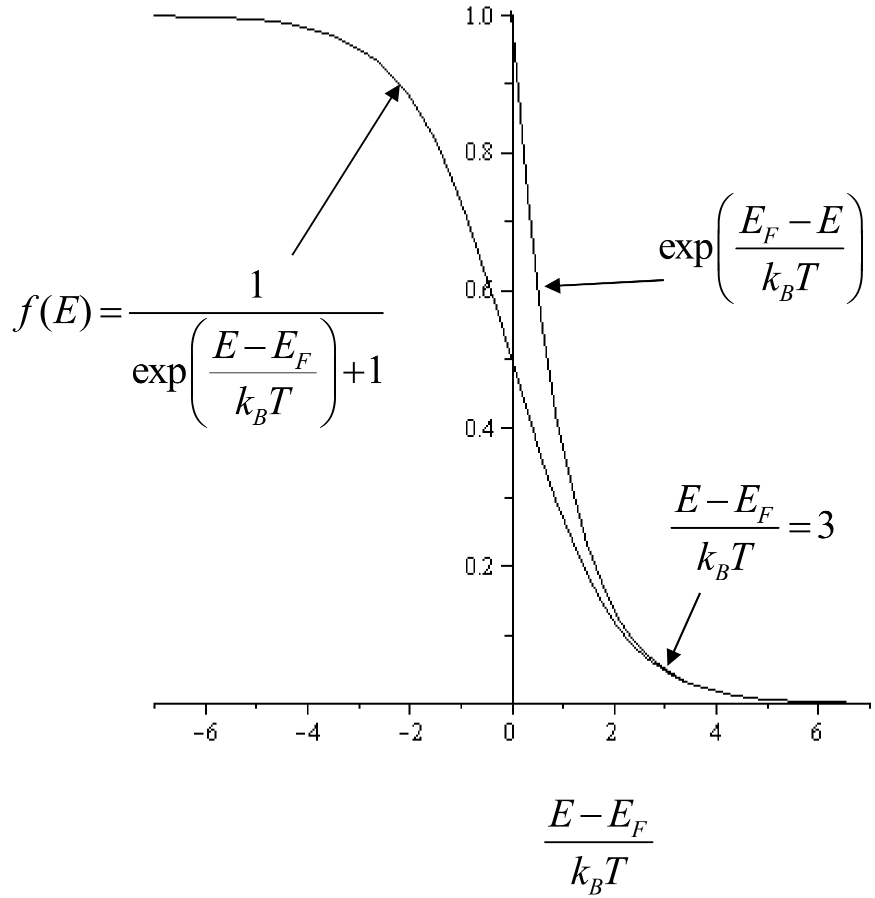




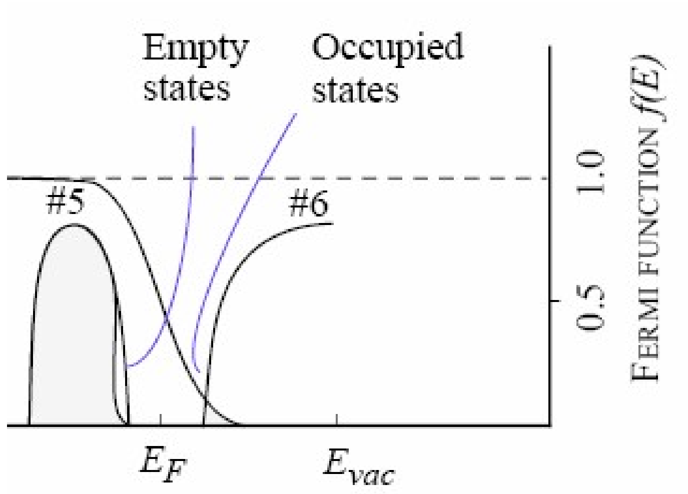




Boltzmann approximation



Density of electrons in the conduction band



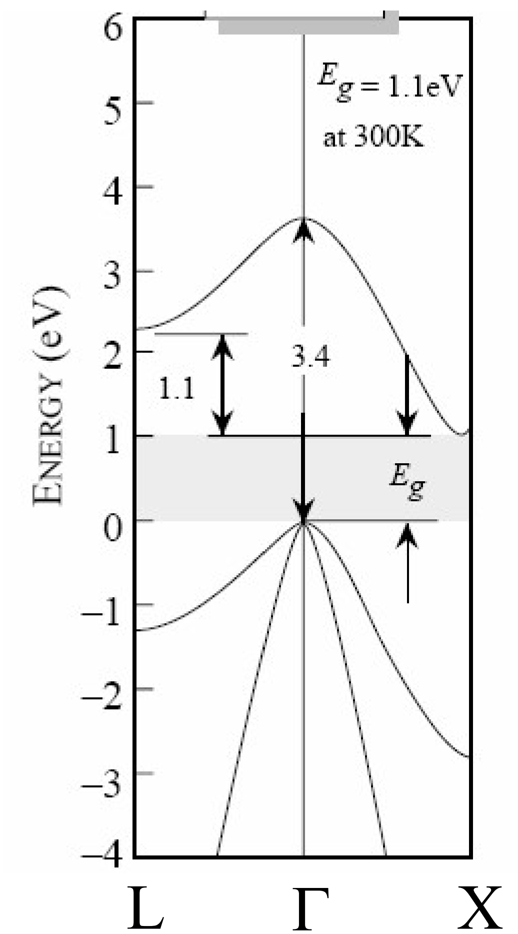
$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx \frac{\pi}{2}\left(\frac{2m^*}{\hbar^2 \pi^2}\right)^{3/2} \int_{E_c}^{\infty} \exp\left(\frac{E_F - E}{k_B T}\right)\sqrt{E - E_c}\, dE$$

$$\frac{\sqrt{\pi}}{2} = \int_0^{\infty} \sqrt{x} e^{-x} dx$$

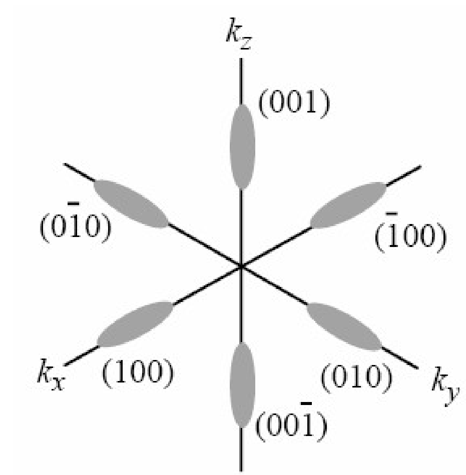
$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

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

Density of electrons in the conduction band



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



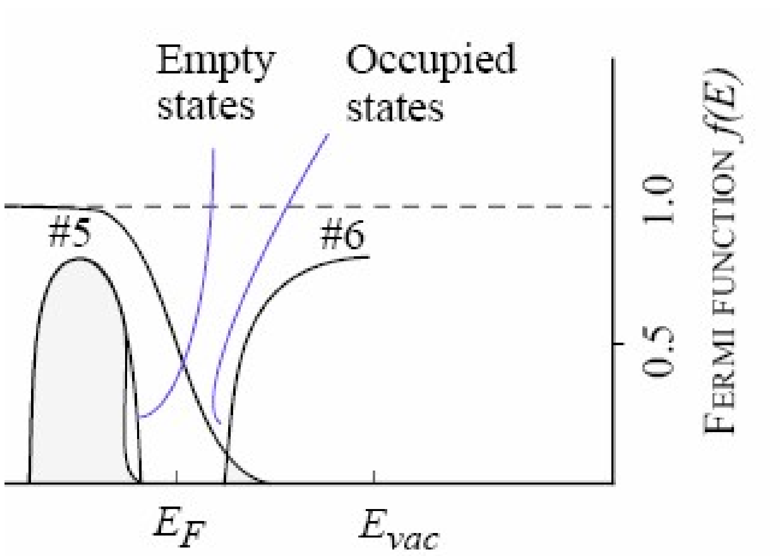
$$n = N_c\left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

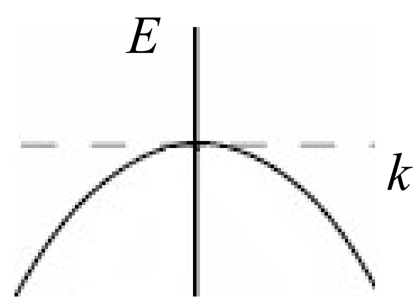
Properties	**Si**	**Ge**	**GaAs**
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}

Density of holes in the valence band

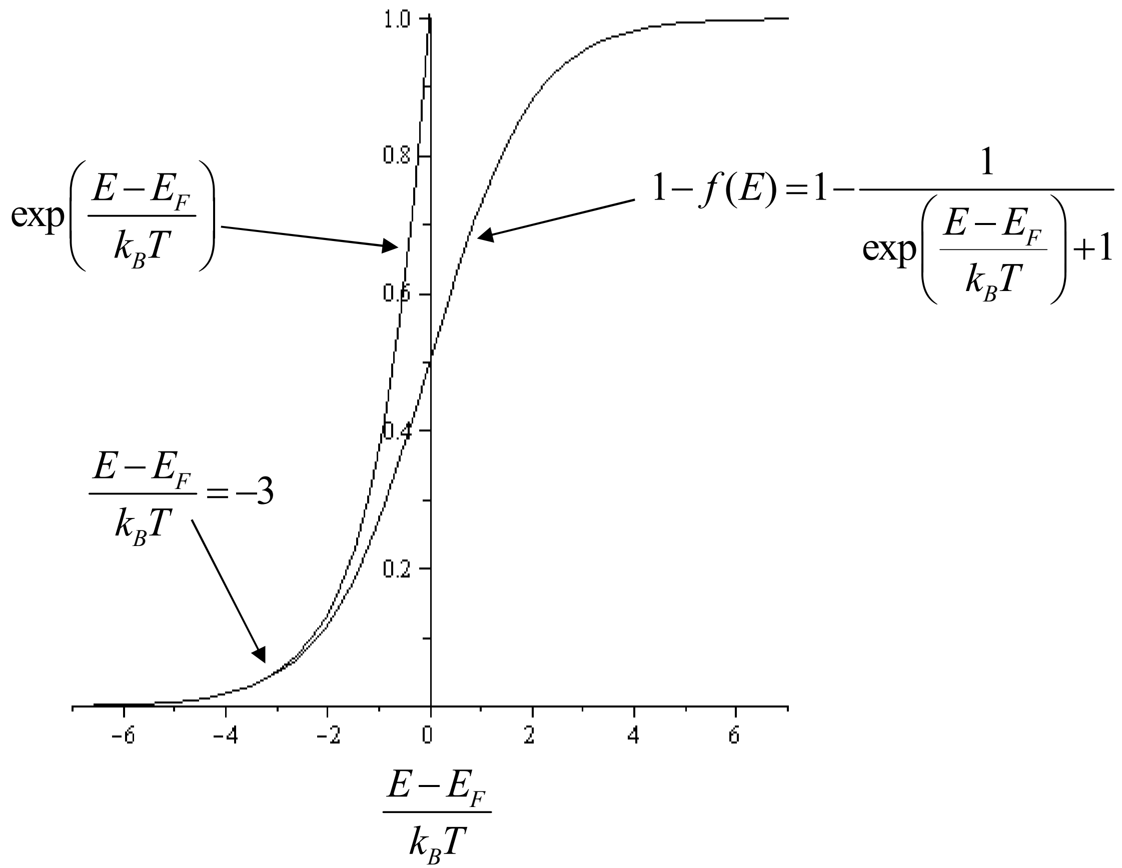
$$D(E) = \frac{\pi}{2}\left(\frac{2m_h^* L^2}{\hbar^2 \pi^2}\right)^{3/2} \sqrt{E_v - E}$$

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

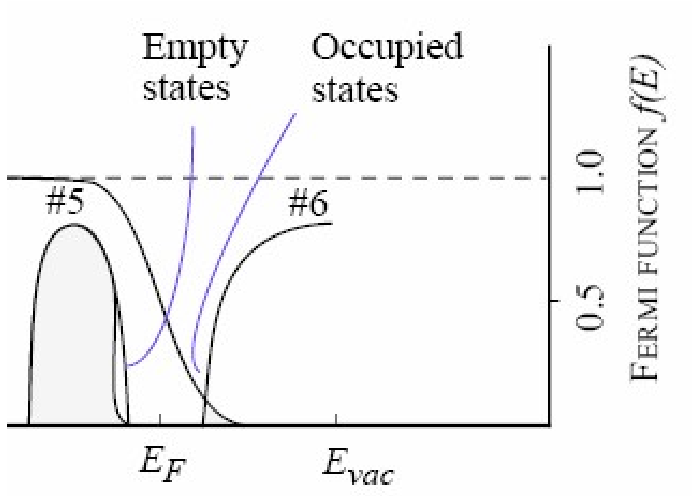




Boltzmann approximation



Density of holes in the valence band



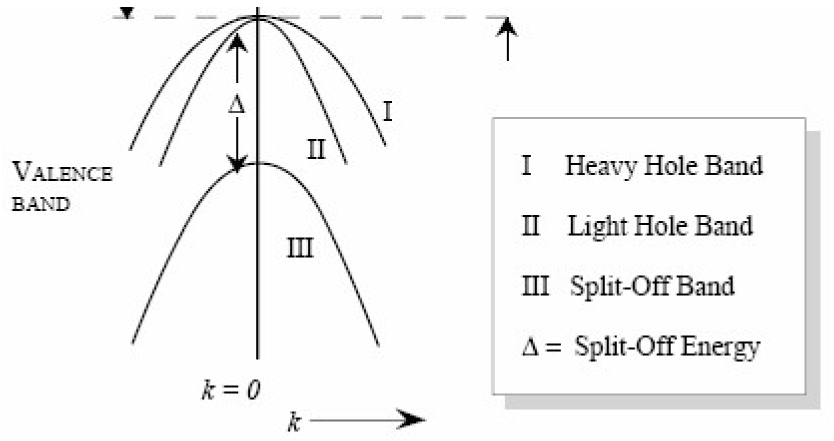
$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right) dE \approx \frac{\pi}{2}\left(\frac{2m_h^*}{\hbar^2\pi^2}\right)^{3/2} \int_{-\infty}^{E_v} \exp\left(\frac{E - E_F}{k_B T}\right)\sqrt{E_v - E}\, dE$$

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

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

= Effective density of states in the valence band

Density of holes in the valence band



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

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

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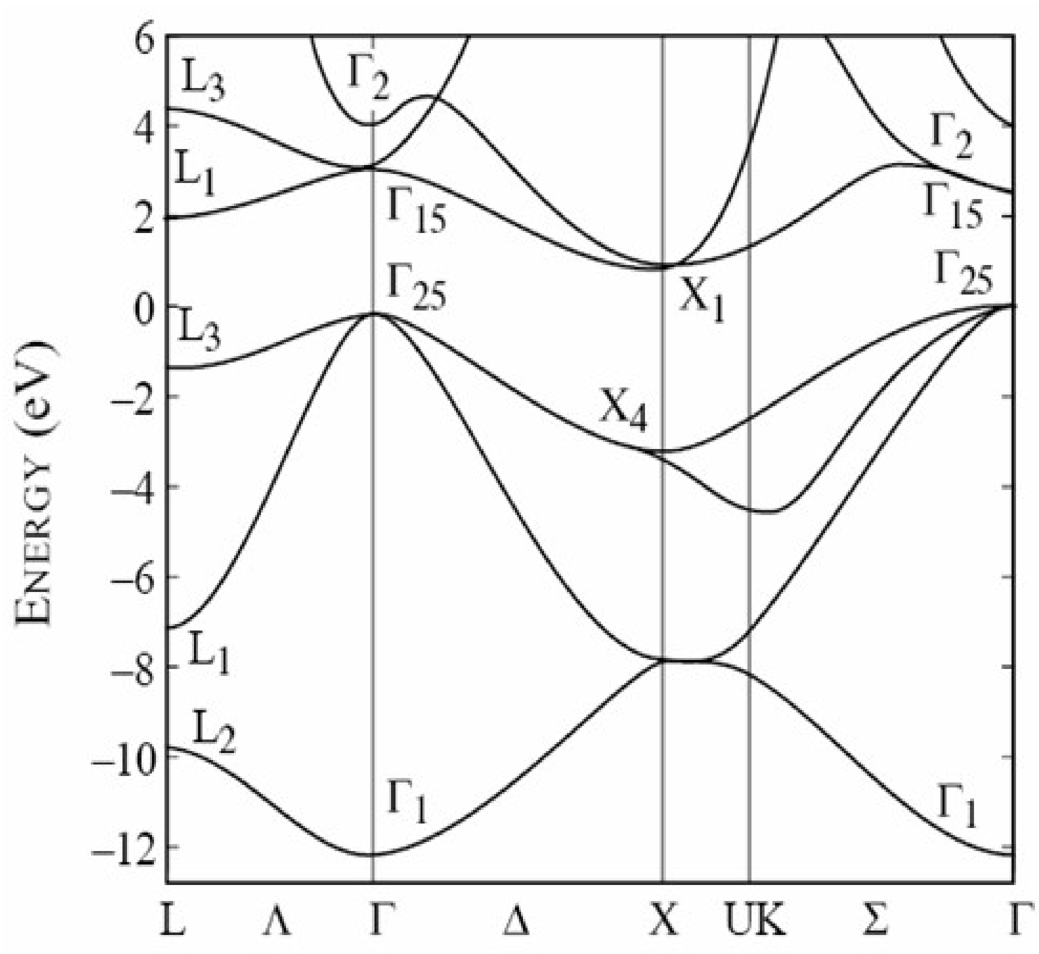
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}
Effective density of states in valence band (300 K) N_v	9.84×10^{24} m^{-3}	6.0×10^{24} m^{-3}	7.72×10^{24} m^{-3}
Effective mass electrons m^*/m_0	$m_l^* = 0.98$ $m_t^* = 0.19$	$m_l^* = 1.64$ $m_t^* = 0.082$	$m^* = 0.067$
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/cm³	5.3267 g/cm³	5.32 g/cm³
Atoms/m³	5.0×10^{28}	4.42×10^{28}	4.42×10^{28}

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.



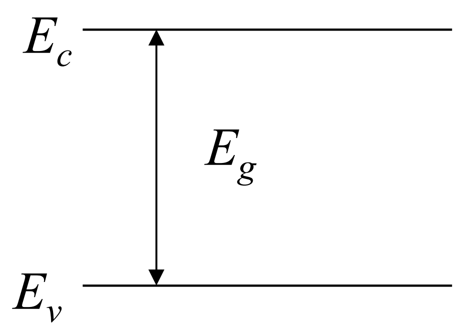
(a) Is this a direct or an indirect semiconductor? Why?

(b) What is the band gap?

(c) 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

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



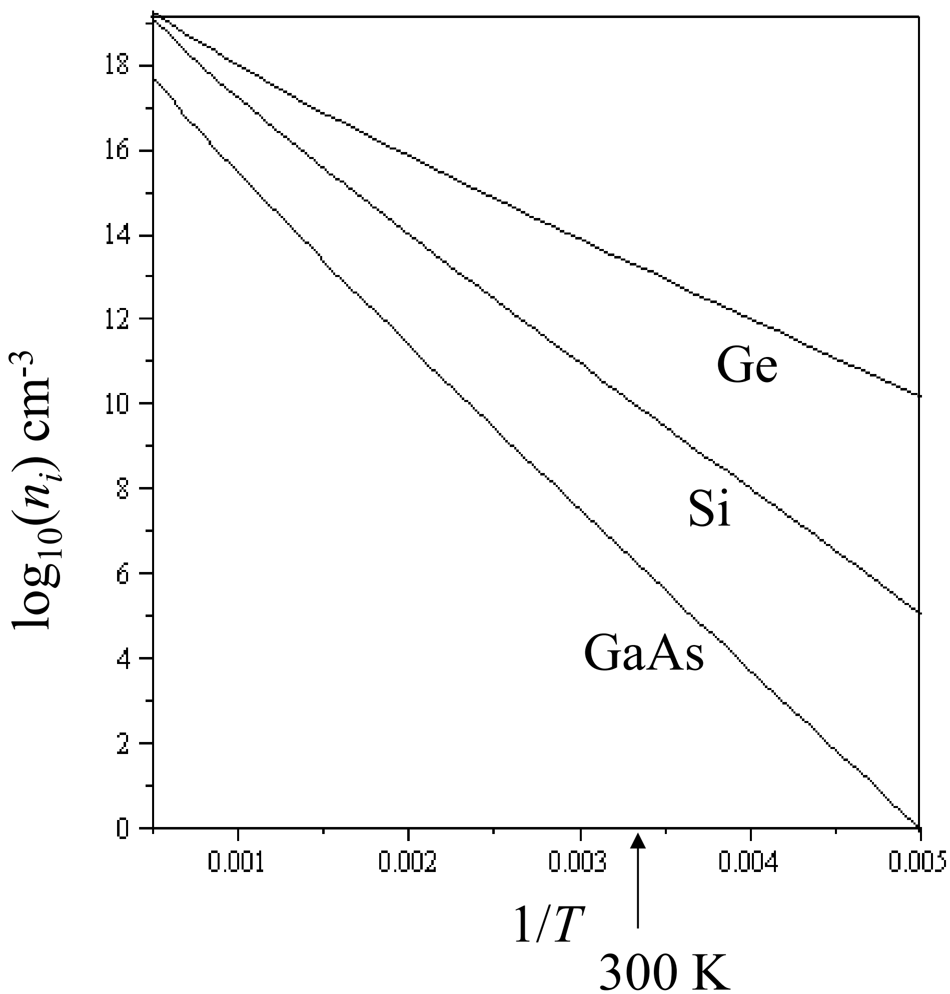
$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

Intrinsic carrier concentration



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

Silicon has ~ 5×10^{22} atoms/cm^3

Good for thermometer, bad for designing circuits.

Fermi energy of an intrinsic semiconductor

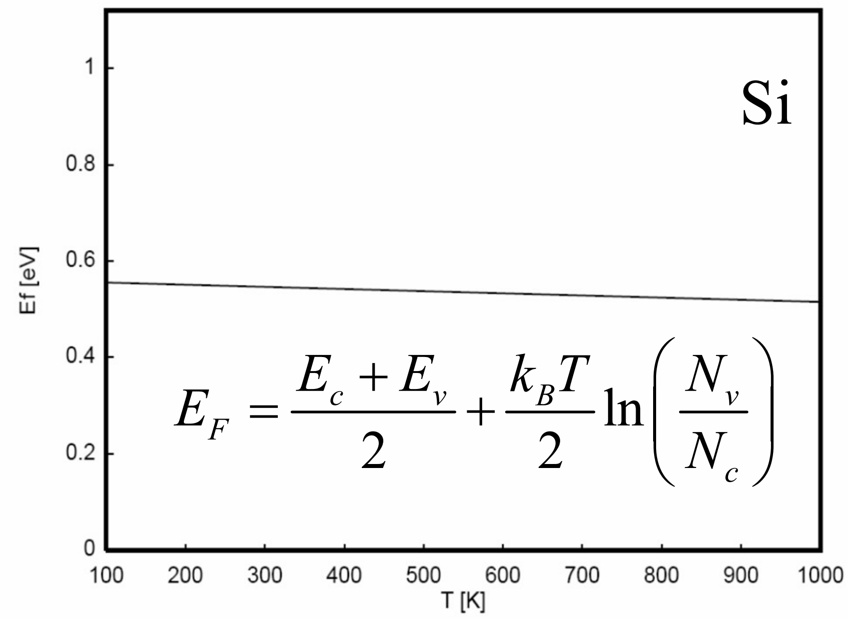
$$n = p = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

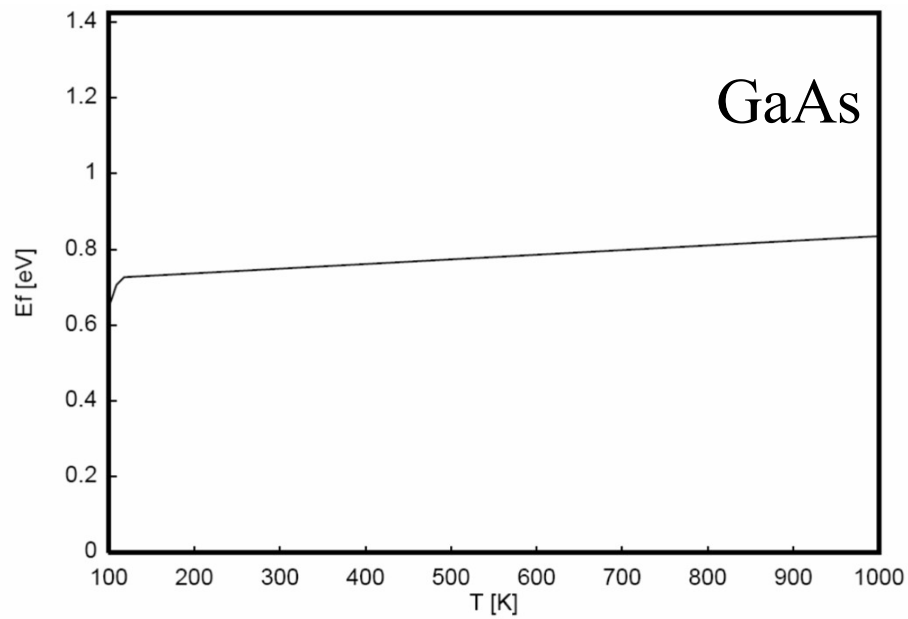
$$\frac{2E_F}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

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

Temperature dependence of E_F



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



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