MSE 423 Fall 2024 – Week 12

Semi-conductors



Last week

- Fermi surfaces
- Group velocity, effective mass
- The independent-electron gas: BvK boundary conditions and the counting of states
- Particles density and energy density
- Density of states; massive vs massless bands
- Statistics of classical and quantum particles
- Probability and partition function
- Chemical potential and Fermi-Dirac distribution

Tight-binding (LCAO for solids)

- Hamiltonian $\hat{H} = \hat{H}_{at} + \Delta\hat{U}\left(\vec{r}\right)$

Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

$$\Psi_{n\vec{k}}\left(\vec{r}\right) = \sum_{\vec{R}} \exp\left(i\vec{k}\bullet\vec{R}\right)\varphi_n\left(\vec{r}-\vec{R}\right)$$

Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

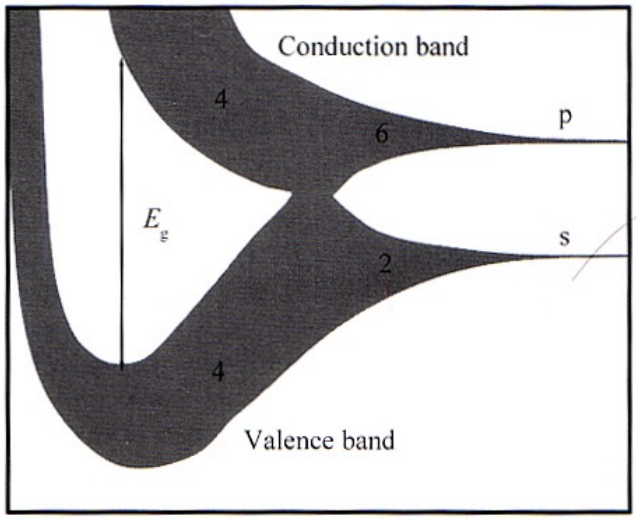
$$\Psi_{n\vec{k}}\left(\vec{r}\right)=\sum_{\vec{R}}\exp\left(i\vec{k}\bullet\vec{R}\right)\phi\left(\vec{r}-\vec{R}\right)$$

$$\phi\left(\vec{r}\right)=\sum_{n}b_{n}\varphi_{n}\left(\vec{r}\right)$$

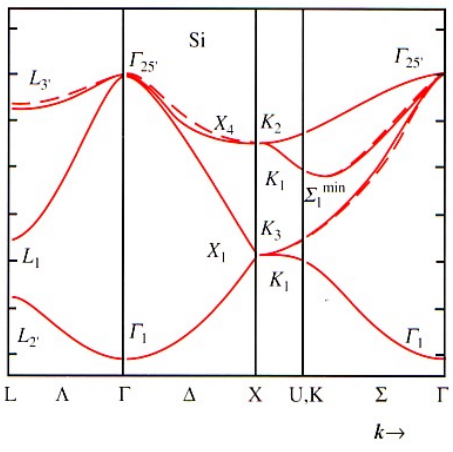
From levels to bands

$$\varepsilon\left(\vec{k}\right)=E_{m}-\beta-\sum_{\substack{nearest\\neighb.}}\gamma\left(\vec{R}\right)\cos\left(\vec{k}\bullet\vec{r}\right)$$

From levels to bands



How many bands in silicon ?



Tight-binding vs. empirical psp

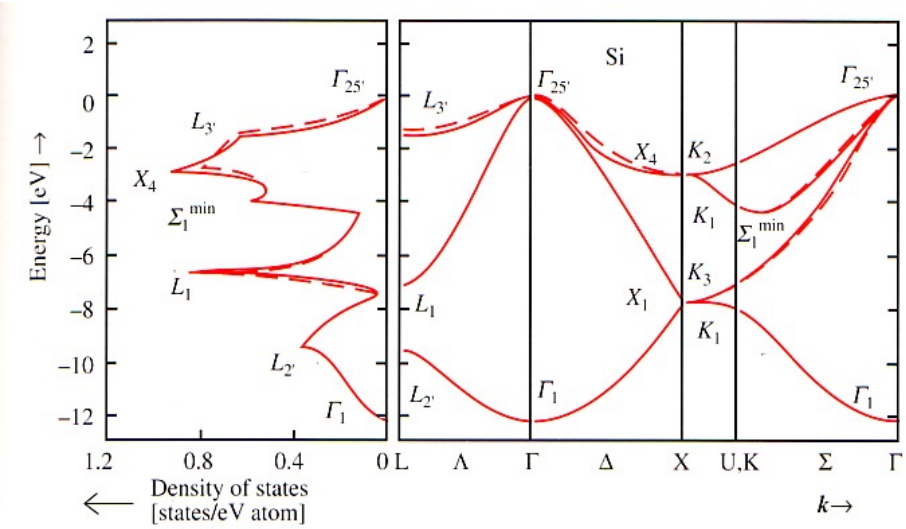


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

Tight-binding vs. empirical psp

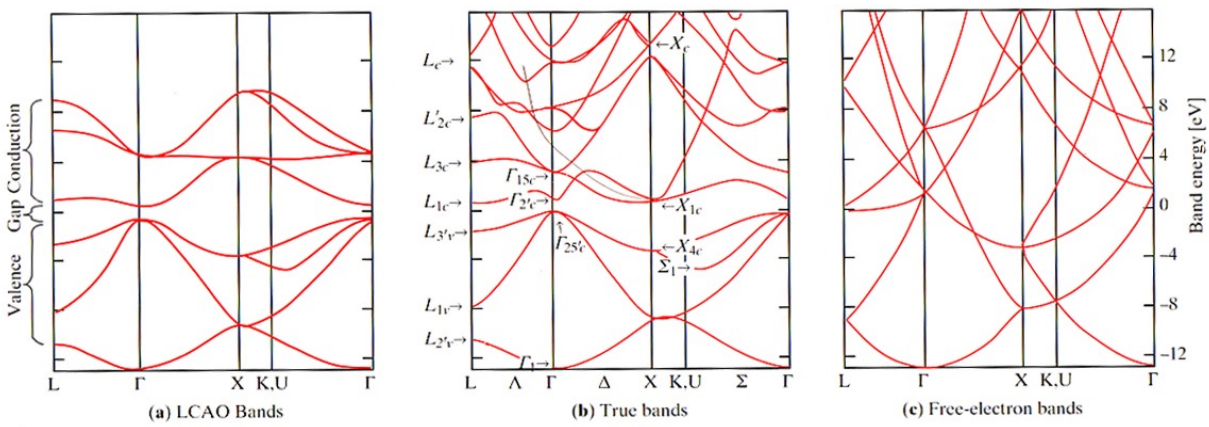
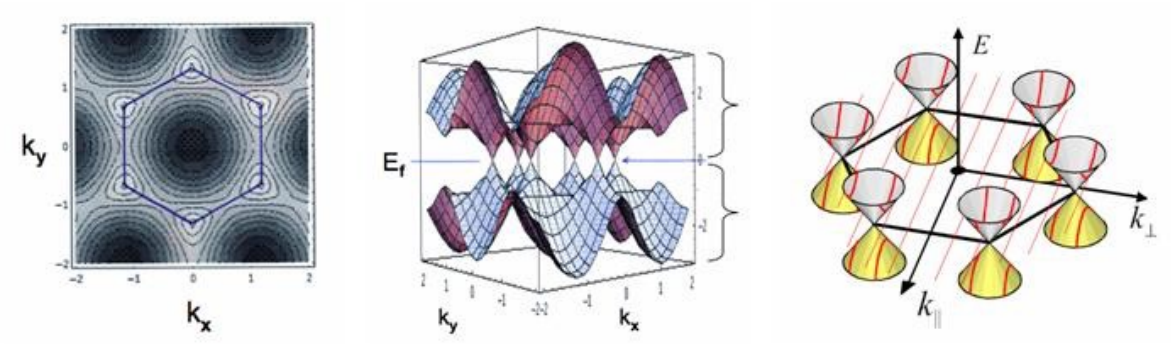
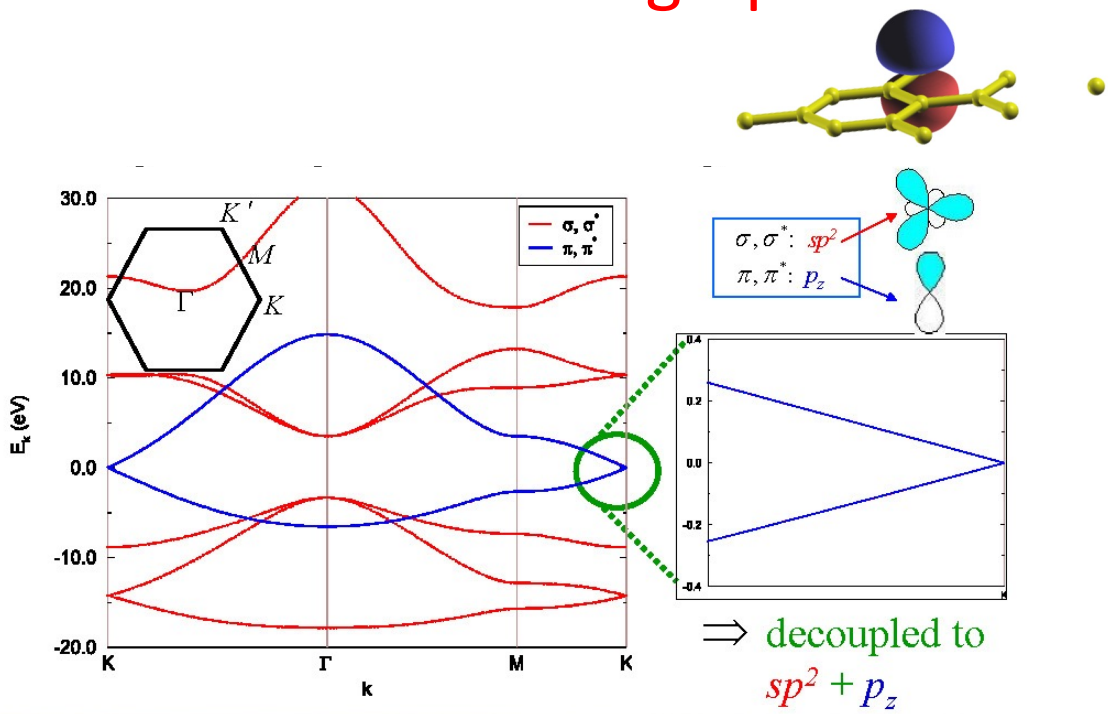


Fig. 2.25. A comparison between the band structure of Ge calculated by **(a)** the tight-binding method, **(b)** the empirical pseudopotential method, and **(c)** the nearly free electron model [Ref. 2.18, p. 79]

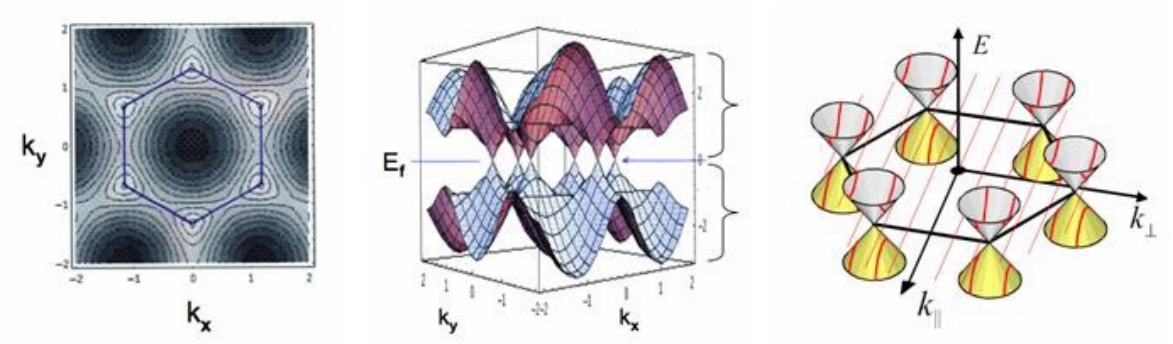
Band structure of graphene



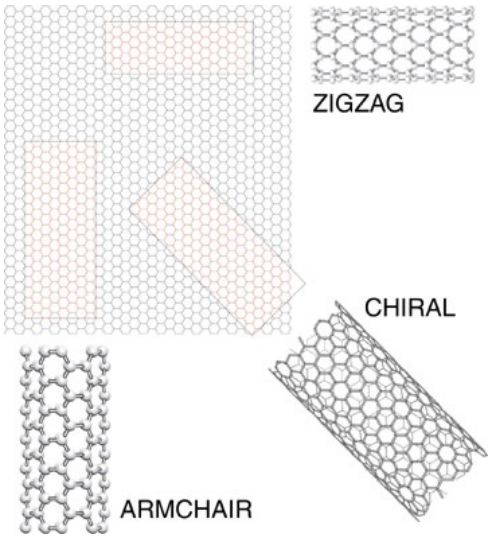
Band structure of graphene



Band structure of graphene

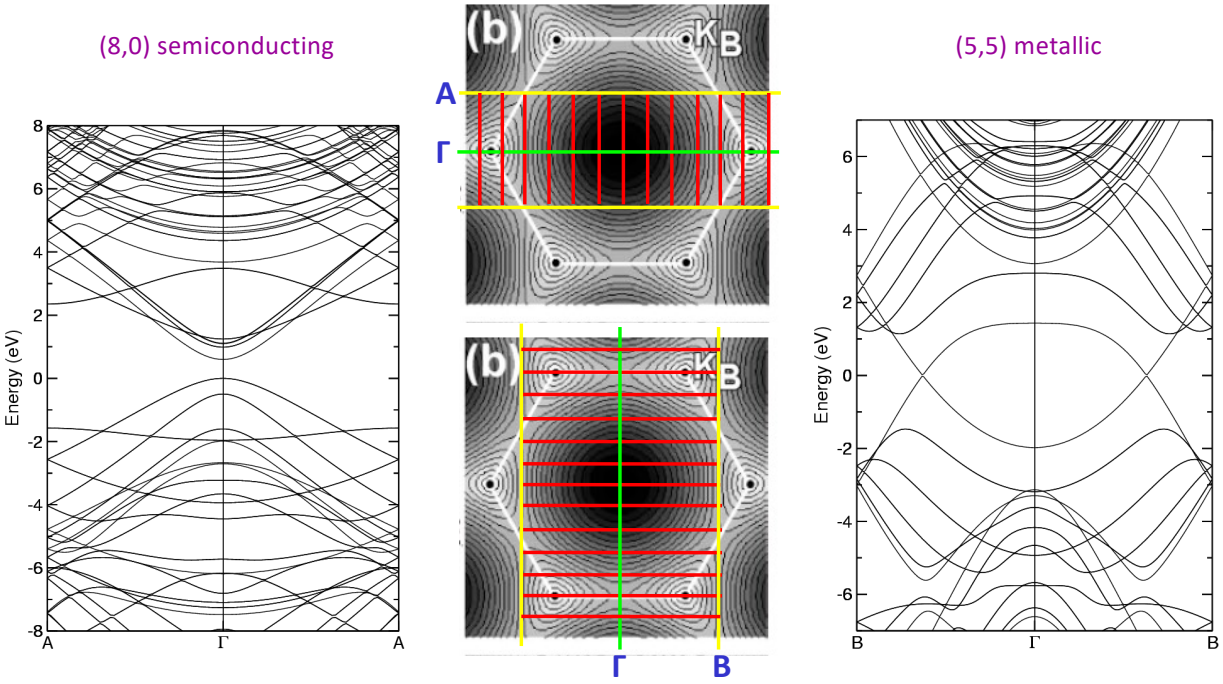


Carbon nanotubes



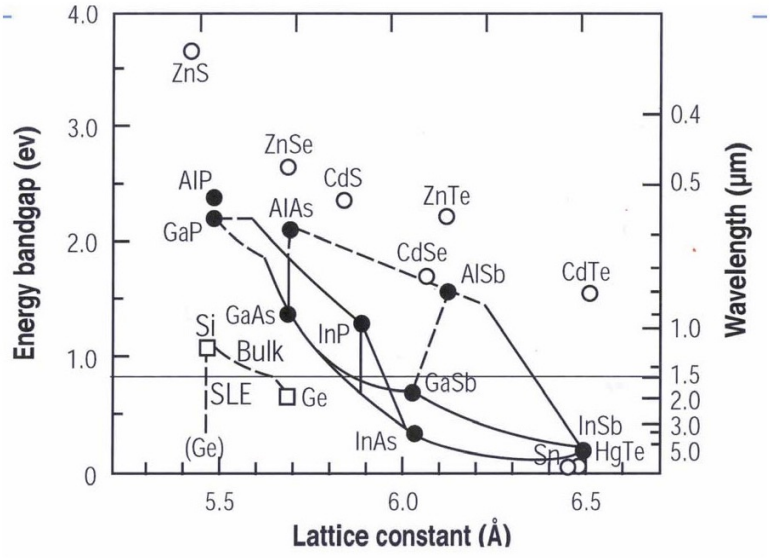
Zone folding: Band structure of nanotubes

(8,0) semiconducting



(5,5) metallic

Semiconductors



Sb-doped Germanium

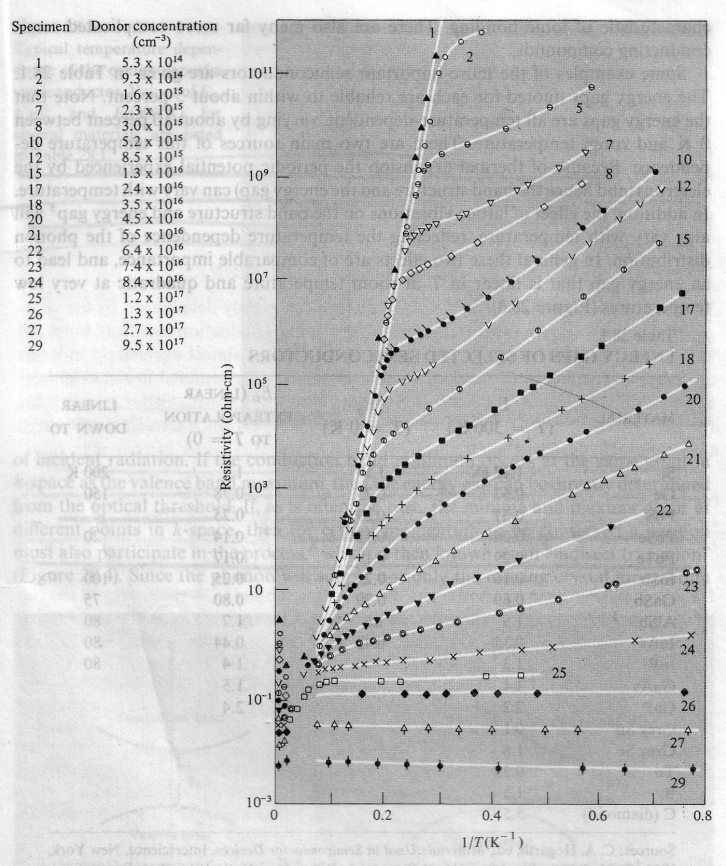
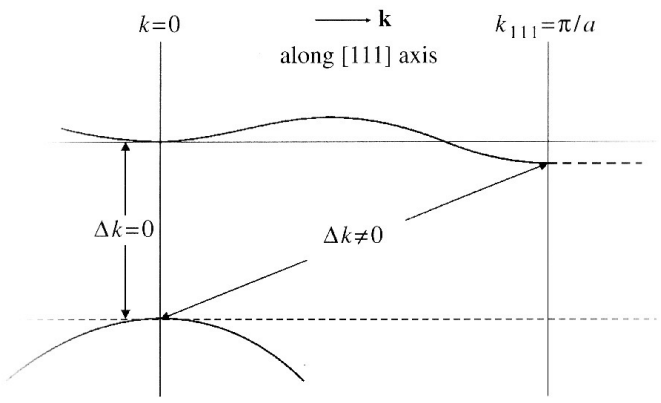
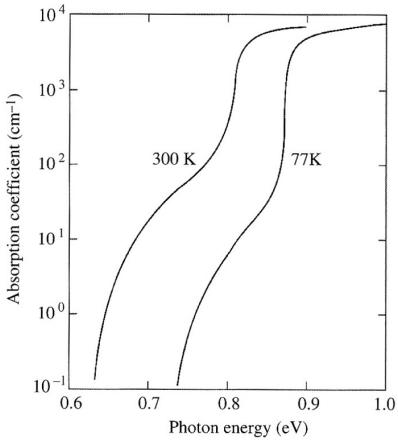


Figure 28.2
The resistivity of antimony-doped germanium as a function of $1/T$ for several impurity concentrations. (From H. J. Fritzsche, *J. Phys. Chem. Solids* **6**, 69 (1958).)

Optical absorption in Ge





Density of carriers at thermal equilibrum

$$n_c(T) = \int_{\epsilon_c}^{\infty} d\epsilon \; g_c(\epsilon) \frac{1}{e^{(\epsilon-\mu)/k_B T}+1}$$

$$p_v(T) = \int_{-\infty}^{\epsilon_v} d\epsilon \; g_v(\epsilon) \left(1 - \frac{1}{e^{(\epsilon-\mu)/K_B T}+1}\right)$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon \; g_v(\epsilon) \left(\frac{1}{e^{(\mu-\epsilon)/K_B T}+1}\right)$$

$$\frac{1}{e^{(\epsilon-\mu)/K_B T}+1} \approx e^{-(\epsilon-\mu)/K_B T}, \; \epsilon > \epsilon_c$$

$$\frac{1}{e^{(\mu-\epsilon)/K_B T}+1} \approx e^{-(\mu-\epsilon)/K_B T}, \; \epsilon < \epsilon_v$$

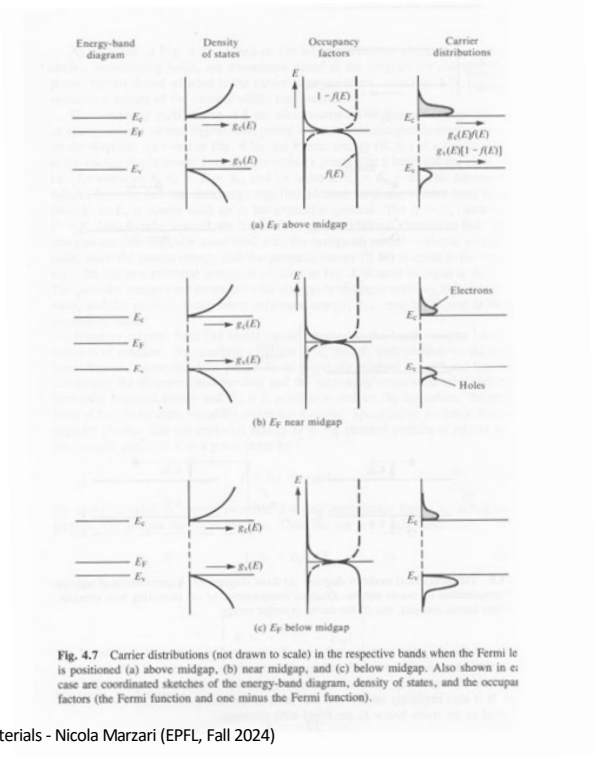


Fig. 4.7 Carrier distributions (not drawn to scale) in the respective bands when the Fermi le is positioned (a) above midgap, (b) near midgap, and (c) below midgap. Also shown in e case are coordinated sketches of the energy-band diagram, density of states, and the occupa factors (the Fermi function and one minus the Fermi function).

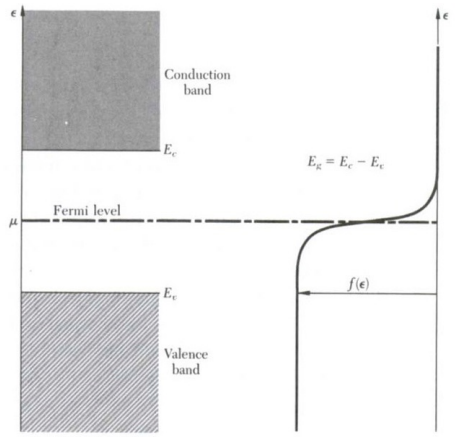
Density of carriers at thermal equilibium
(non-degenerate sc)

$$n_c(T) = \int_{\epsilon_c}^{\infty} d\epsilon \; g_c(\epsilon) \frac{1}{e^{(\epsilon-\mu)/k_B T}+1}$$

$$\approx \int_{\epsilon_c}^{\infty} d\epsilon \; g_c(\epsilon) e^{-(\epsilon-\mu)/k_B T}$$

$$= \left\{ \int_{\epsilon_c}^{\infty} d\epsilon \; g_c(\epsilon) e^{-(\epsilon-\epsilon_c)/k_B T} \right\} e^{-(\epsilon_c-\mu)/k_B T}$$

$$= N_c(T) e^{-(\epsilon_c-\mu)/k_B T}$$



$$p_v(T) = \int_{-\infty}^{\epsilon_v} d\epsilon \; g_v(\epsilon) \left(1 - \frac{1}{e^{(\epsilon-\mu)/k_B T}+1}\right) = ... = P_v(T) e^{-(\mu-\epsilon_v)/k_B T}$$

Density of available states (isotropic effective mass)

$$g_{c,v}(\epsilon) = \sqrt{2|\epsilon - \epsilon_{c,v}|}\frac{m_{c,v}^{3/2}}{\hbar^3\pi^2}$$

$$N_c(T) = \int_{\epsilon_c}^{\infty} d\epsilon\ g_c(\epsilon)e^{-(\epsilon-\epsilon_c)/K_BT}$$

$$P_v(T) = \int_{-\infty}^{\epsilon_v} d\epsilon\ g_v(\epsilon)e^{-(\epsilon_v-\epsilon)/K_BT}$$

$$N_c(T) = \frac{1}{4}\left(\frac{2m_c k_B T}{\pi\hbar^2}\right)^{3/2} \qquad N_c(T) = 2.5\left(\frac{m_c}{m}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2} 10^{19}\ /\ cm^3$$

$$P_v(T) = \frac{1}{4}\left(\frac{2m_v k_B T}{\pi\hbar^2}\right)^{3/2} \qquad P_v(T) = 2.5\left(\frac{m_v}{m}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2} 10^{19}\ /\ cm^3$$

Miracle! Law of Mass Action

$$n_c(T) = N_c(T)e^{-(\epsilon_c-\mu)/K_BT}$$

$$p_v(T) = P_v(T)e^{-(\mu-\epsilon_v)/K_BT}$$

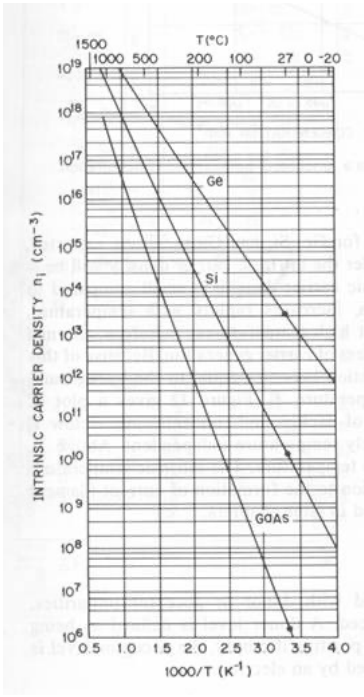
$$n_c(T)p_v(T) = N_c(T)P_v(T)e^{-\frac{(\epsilon_c-\epsilon_v)}{K_BT}}$$

$$= N_c(T)P_v(T)e^{-\frac{E_{gap}}{K_BT}}$$

This is a property of the material (does not depend on doping)

Intrinsic case

$$n_c(T) = p_v(T) \equiv n_i(T)$$



$$n_i = \sqrt{n_c p_v} = \sqrt{N_c P_v} e^{-E_g/2k_BT}$$

$$= 2.5 \left(\frac{m_c}{m}\right)^{\frac{3}{4}} \left(\frac{m_v}{m}\right)^{\frac{3}{4}} \left(\frac{T}{300K}\right)^{\frac{3}{2}} e^{-\frac{E_g}{2K_BT}} \; 10^{19}/cm^3$$

Intrinsic case

$$n_c(T) = N_c(T) e^{-(\epsilon_c - \mu)/K_BT}$$

$$p_v(T) = P_v(T) e^{-(\mu - \epsilon_v)/K_BT}$$

$$1 = \frac{n_c(T)}{p_v(T)} = \frac{N_c(T)}{P_v(T)} e^{2\mu/K_BT} e^{(2\epsilon_v + E_g)/K_BT}$$

$$\mu = \mu_i = \epsilon_v + \frac{E_g}{2} + \frac{k_BT}{2} \ln \frac{P_v(T)}{N_c(T)}$$

$$= \epsilon_v + \frac{E_g}{2} + \frac{3}{4} K_BT \ln \left(\frac{m_v}{m_c}\right)$$