MSE 423 Fall 2024 – Week 12

Semi-conductors

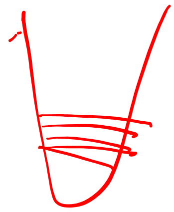
Last week

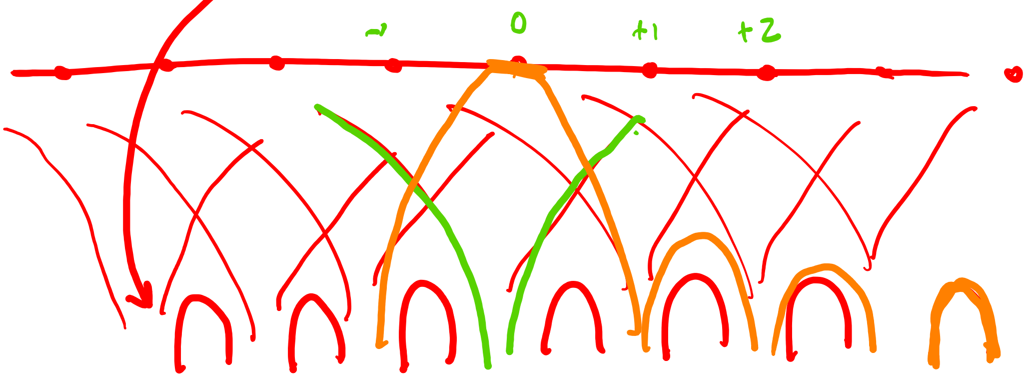
$\varepsilon_n(\vec{k}) = \varepsilon_F$

- 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 (k^2) vs massless (k) bands
- Statistics of classical (dist.) and quantum (indist.) particles
- Probability and partition function
- Chemical potential and Fermi-Dirac distribution

Tight-binding (LCAO for solids)

- Hamiltonian $\hat{H} = \hat{H}^{0}_{at} + \Delta\hat{U}(\vec{r})$





Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

BLOCH SUM ATOMIC ORBITAL

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

A BLOCH SUM SATISFIES BLOCH THEOREM

$$\Psi_{n\vec{k}}(\vec{r}+\vec{R}) = \sum_{\vec{R}'} \exp(i\vec{k}\cdot\vec{R}')\,\varphi_n(\vec{r}-\vec{R}'+\vec{R})$$

$$= \sum_{\vec{R}'} e^{i\vec{k}\cdot\vec{R}'} e^{i\vec{k}\cdot\vec{R}} \cdot e^{-i\vec{k}\cdot\vec{R}}\,\varphi_n(\vec{r}-\vec{R}'+\vec{R})$$

$$= e^{i\vec{k}\cdot\vec{R}} \sum_{\vec{R}'} e^{i\vec{k}\cdot(\vec{R}'-\vec{R})}\,\varphi_n(\vec{r}-(\vec{R}'-\vec{R}))$$

$$= e^{i\vec{k}\cdot\vec{R}} \sum_{\vec{R}''} e^{i\vec{k}\cdot\vec{T}}\,\varphi_n(\vec{r}-\vec{T})$$

Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

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

$$\phi(\vec{r}) = \sum_{n} b_n \varphi_n(\vec{r})$$

WANNIER FUNCTIONS

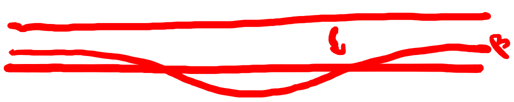
SIMPLE CUBIC LATTICE (α-Po)

From levels to bands

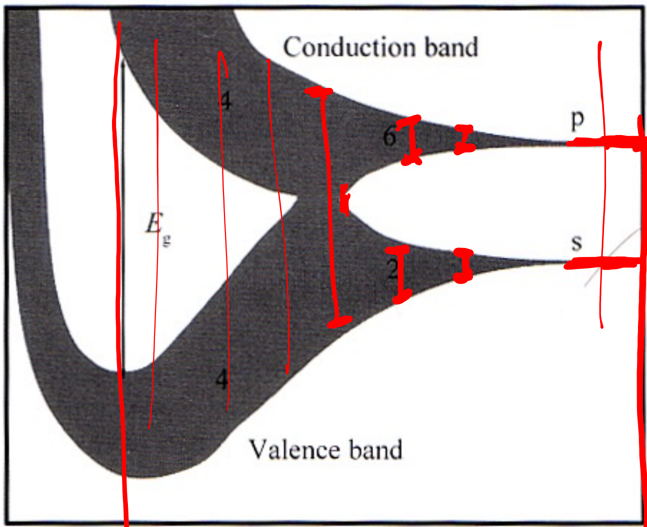
$\beta = -\int \varphi^*(\vec{r})\, \Delta U\, \varphi(\vec{r})$

$\gamma = -\int \varphi^*(\vec{r})\, \Delta U\, \varphi(\vec{r} - \vec{R})$

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



From levels to bands



ATOM A

↑↓ $3p_x$ — $3p_y$ $3p_z$

↑↓ $3p_x$ — $3p_y$ $3p_z$

↑↓ 3s ↑↓ 3s

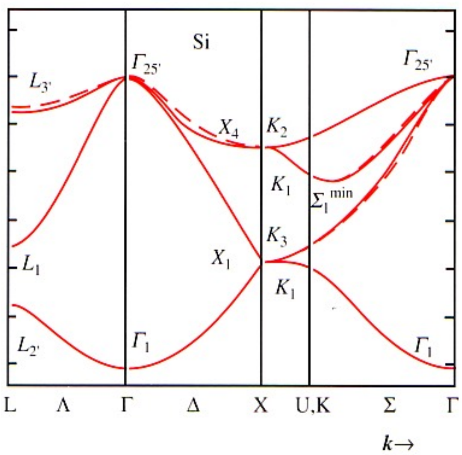
ATOM A ATOM B

2 FLAT BAND

SILICON @ EQ. LATTICE PARAMETER

Si IN THIS EXPLODED ATOMIC LIMIT

How many bands in silicon ?



Tight-binding vs. empirical psp

"TRUTH"

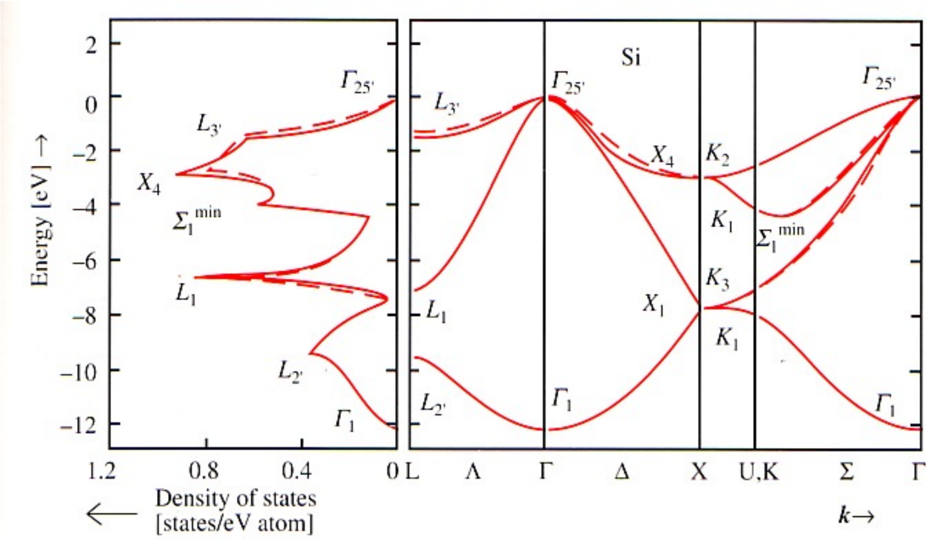


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

Tight-binding vs. empirical psp

8 BANDS FROM SIMPLEST T.B MODEL

"TRUE"

FREE ELECTRON

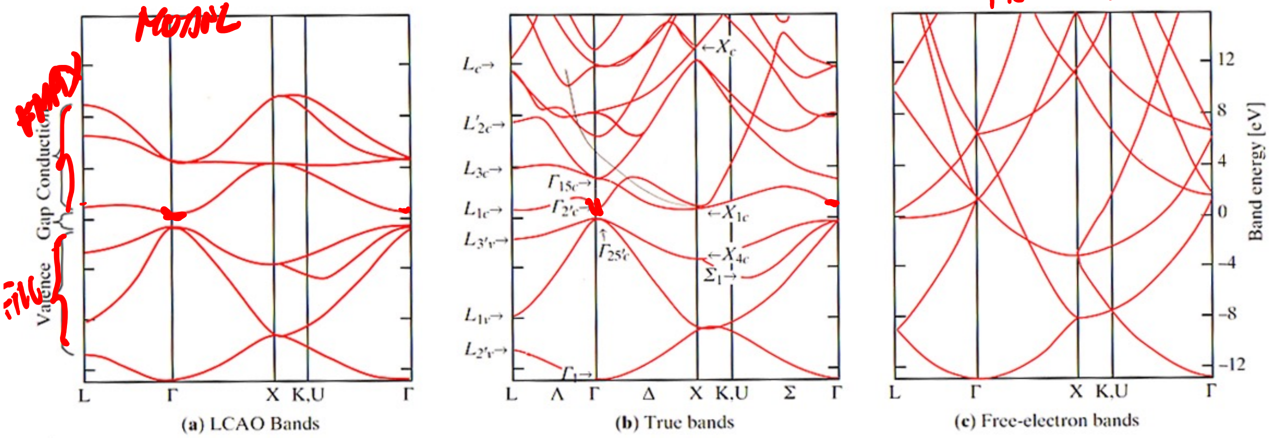


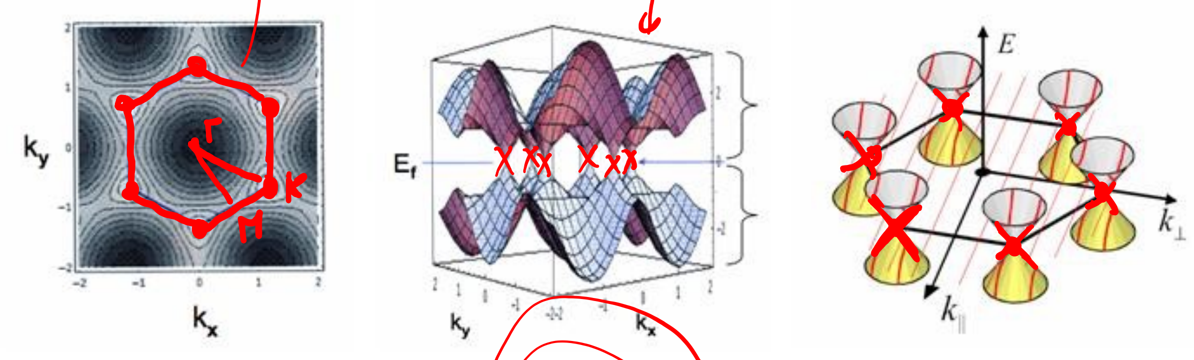
Fig. 2.25. A comparison between the band structure of Ge calculated by (**a**) the tight-binding method, (**b**) the empirical pseudopotential method, and (**c**) the nearly free electron model [Ref. 2.18, p. 79]

Band structure of graphene

BZ OF GRAPHENE

π BANDS

p_z ORBITALS

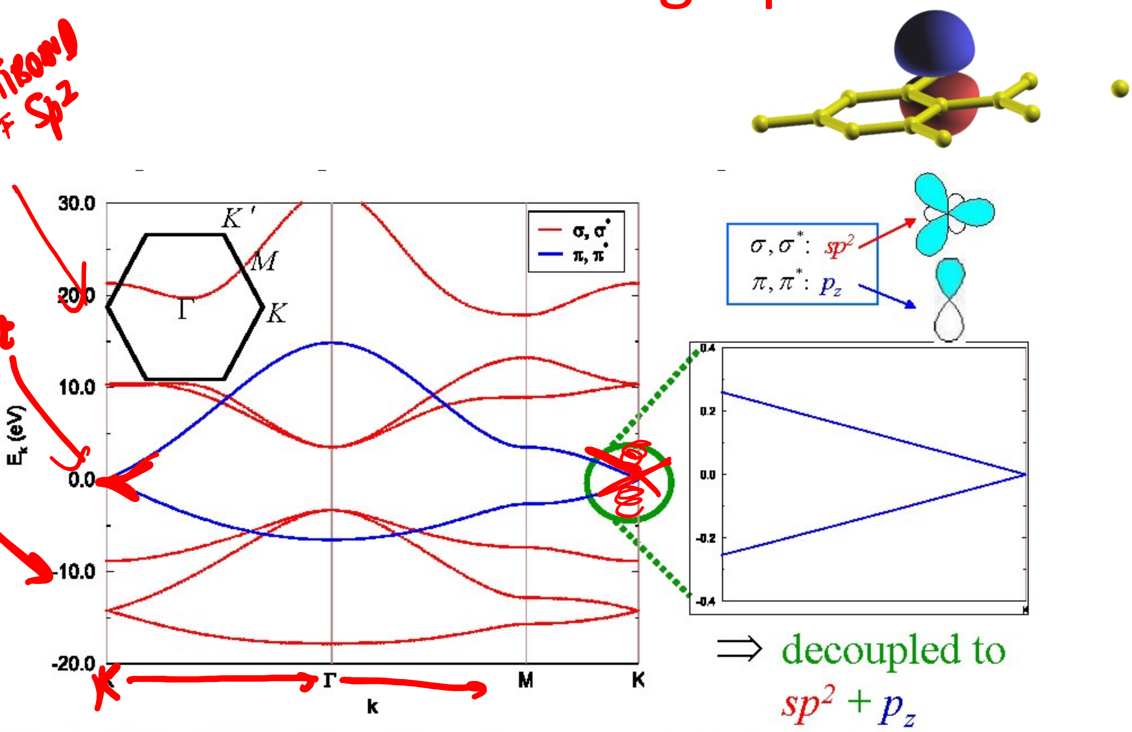


Band structure of graphene

ANTIBOND of sp^2

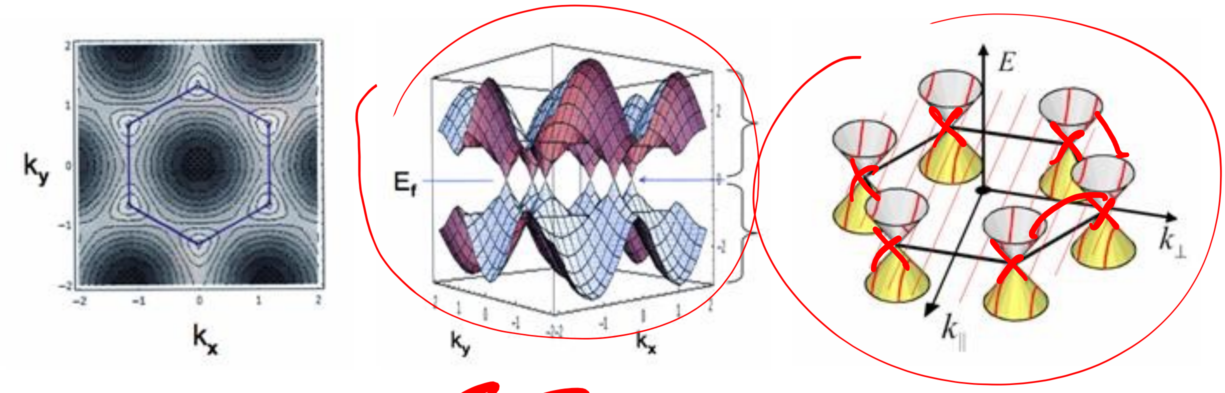
p_z

BOND sp^2

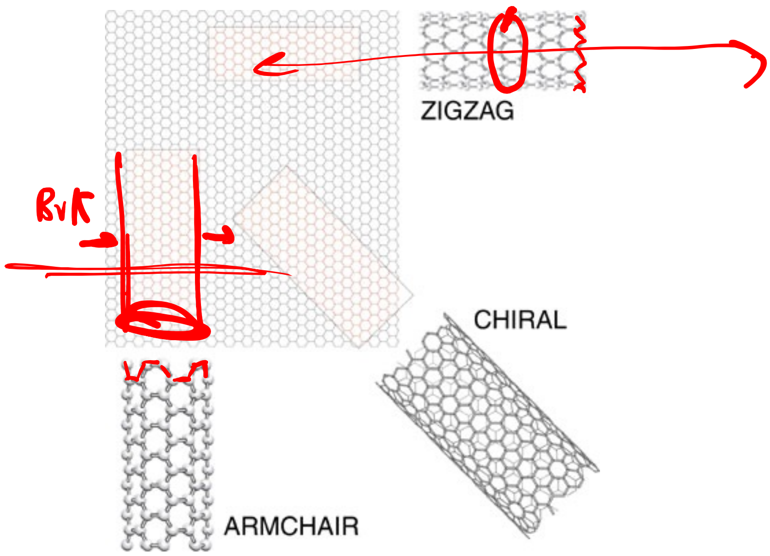


$\Rightarrow$ decoupled to $sp^2 + p_z$

Band structure of graphene

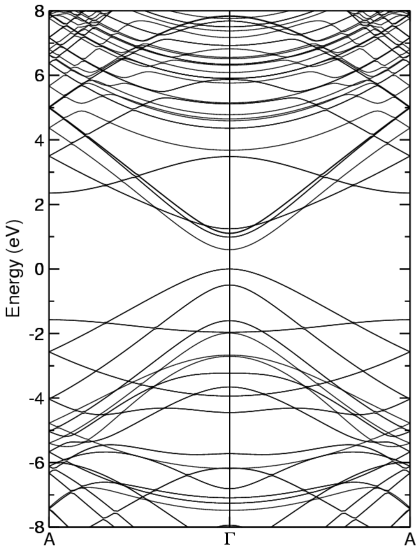


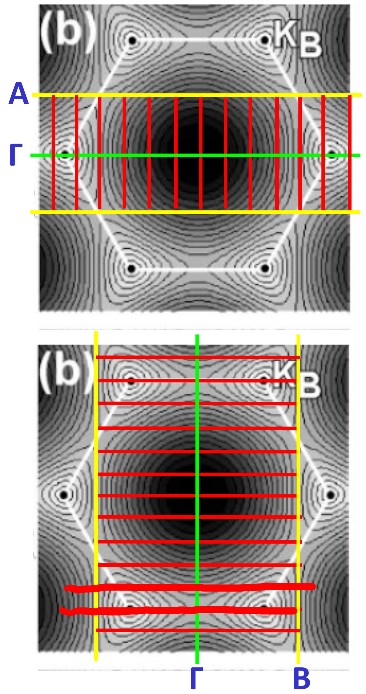
Carbon nanotubes



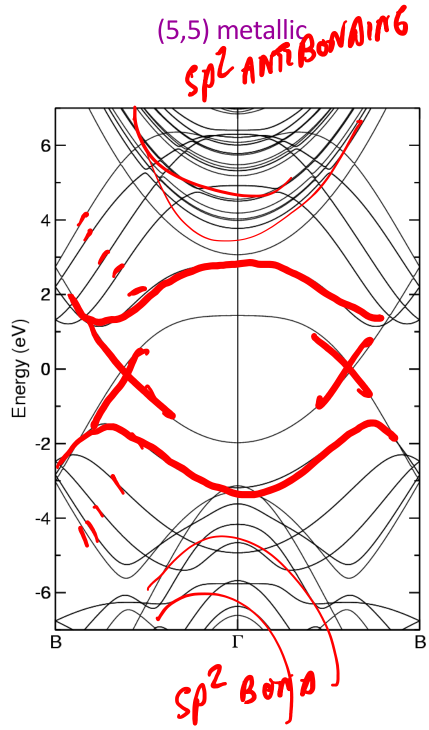
Zone folding: Band structure of nanotubes

(8,0) semiconducting

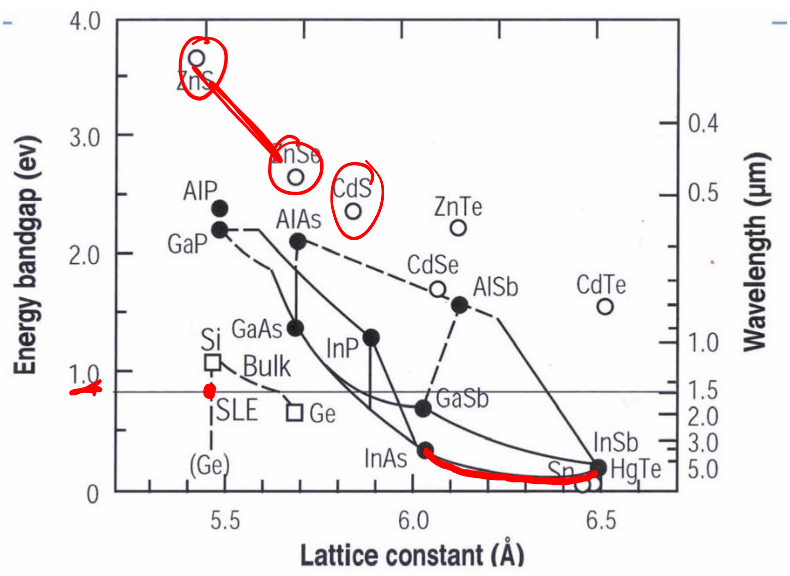




(5,5) metallic



Semiconductors



Sb-doped Germanium

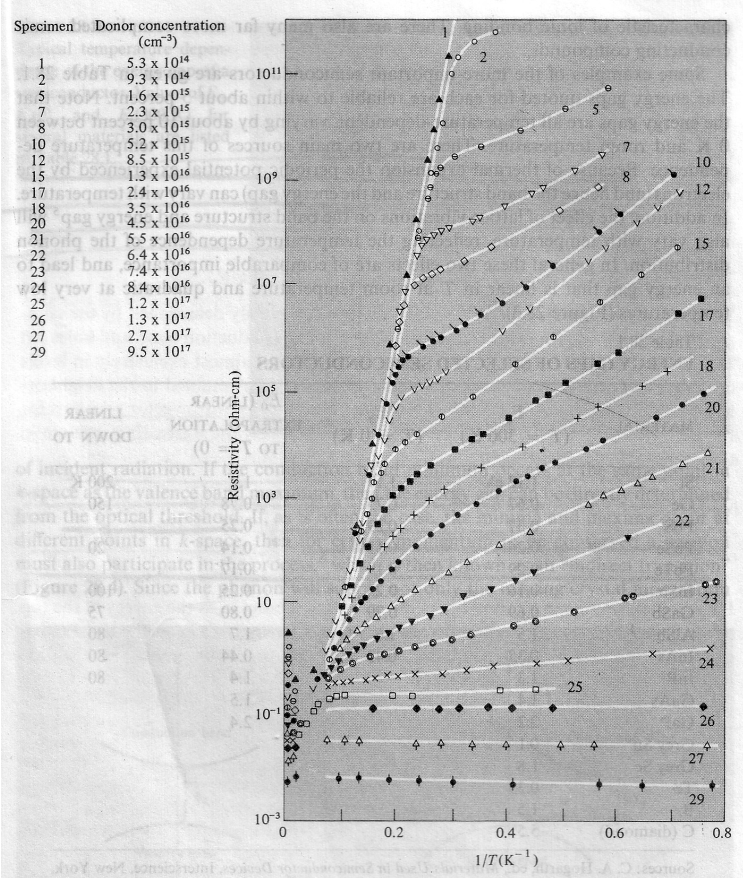
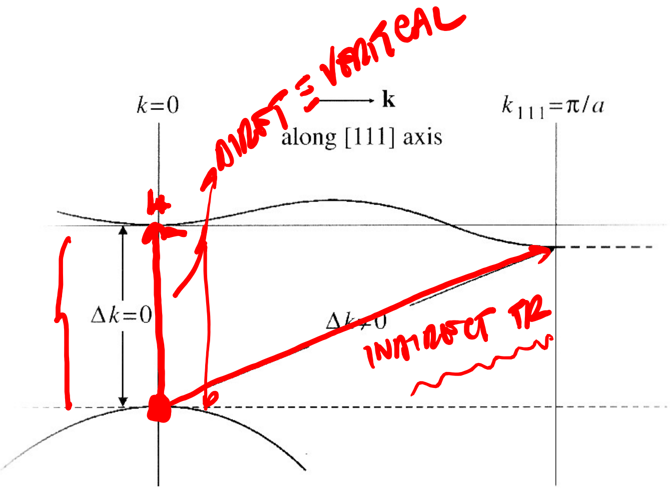
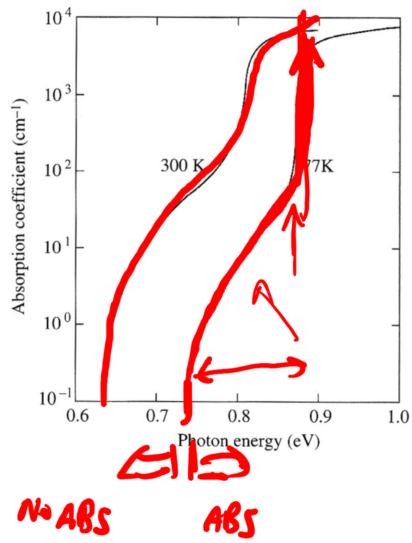


Figure 28.2
The resistivity of antimony-doped germanium as a function of $1/T$ for several impurity concentrations. (From H. J. Fritzsche, *J. Phys. Chem. Solids* **6**, 69 (1958).)

Optical absorption in Ge





Density of carriers at thermal equilibrum

DENS. OF ST

OCCUPATION OF A STATE

ROOM TEMP: 300K $\simeq \frac{1}{40}$ eV (1eV $\simeq$ 11600K)

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

DENS. OF NEG. CARRIERS = ELECTRONS

DENS. OF POS. CARRIERS / VACANCY = HOLES

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

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

NON-DEGENERATE CASE

$$\frac{1}{\underbrace{e^{(\epsilon-\mu)/K_BT}}_{\text{0.5 eV OR MORE}}\cancel{+1}} \approx \underline{e^{-(\epsilon-\mu)/K_BT}},\quad \epsilon > \epsilon_c$$

$$\frac{1}{\underbrace{e^{(\mu-\epsilon)/K_BT}}_{\text{0.5 eV OR LARGER}}\cancel{+1}} \approx \underline{e^{-(\mu-\epsilon)/K_BT}},\quad \epsilon < \epsilon_v$$

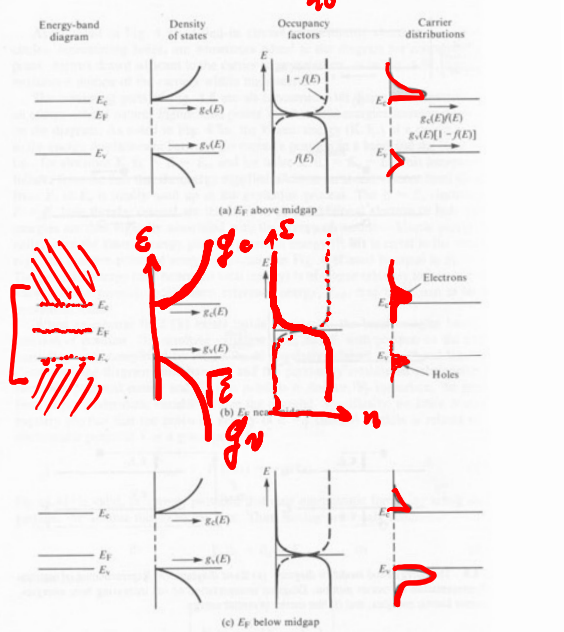


Fig. 4.7 Carrier distributions (not drawn to scale) in the respective bands when the Fermi le is positioned (a) above midgap, (b) near midgap, and (c) below midgap. Also shown in ea case are coordinated sketches of the energy-band diagram, density of states, and the occupar factors (the Fermi function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

Density of carriers at thermal equilibium

(non-degenerate sc)

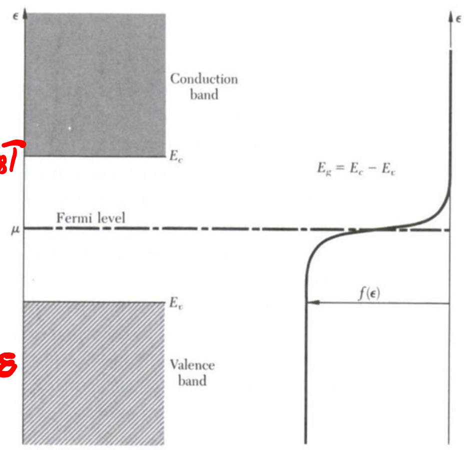
$$n_c(T) = \int_{\epsilon_c}^{\infty} d\epsilon\; g_c(\epsilon)\frac{1}{e^{(\epsilon-\mu)/k_BT}\cancel{+1}}$$

$$\approx \int_{\epsilon_c}^{\infty} d\epsilon\; g_c(\epsilon)e^{-(\epsilon-\mu)/k_BT}\; e^{-\epsilon_c/k_BT}\,e^{+\epsilon_c/k_BT}$$

DENSITY OF AVAILABLE STATES

$$= \underbrace{\left\{\int_{\epsilon_c}^{\infty} d\epsilon\; g_c(\epsilon)e^{-(\epsilon-\epsilon_c)/k_BT}\right\}}\; \underbrace{e^{-(\epsilon_c-\mu)/k_BT}}_{\text{DOES NOT DEP ON }\epsilon}$$

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



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

Density of available states (isotropic effective mass)

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

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

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

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

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

Miracle! Law of Mass Action

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

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

INDEPENDENT OF μ

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

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

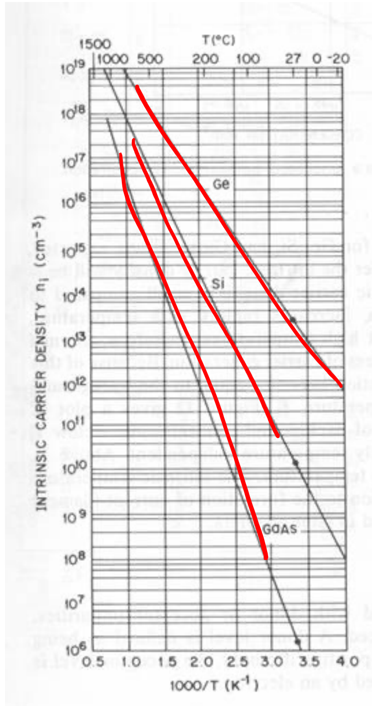
This is a property of the material (does not depend on doping)

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

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

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

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

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

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