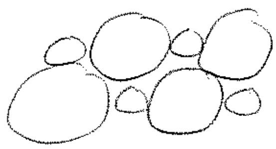
HW STREETMAN CH 2 # 8-11

Streetman Ch 3 + Kittel Ch 7

know e^- are in discrete energy levels
in an atom
in solid → e^- "feel" neighboring atoms
⇒ e^- has a band of allowed energies
forbidden ⇒ band gaps

Bonding
ionic bonds : e^- tightly bound to atoms
Na^+ + Cl^- → e static force



few if any e^- move
about ⇒ insulator

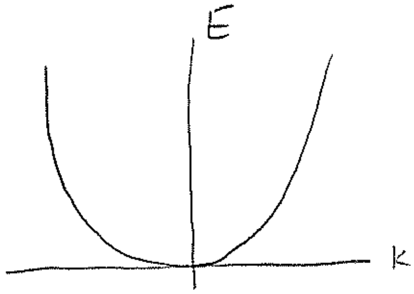
metallic bonds : outer shell less than half
full (e.g. alkalis) ⇒ e^- tend to move
⇒ conductor ; force btwn core + e^-

covalent bonds ; each atom shares valence
e^- w/ its neighbors ; lattice held together
by QM interactions of e^-
both e^- belong to both atoms differ only
in spin
e.g. col IV → should be insulators (C)
⇒ semiconductors

Where does the band gap come from

free e^- model $\rightarrow$ allowed energy levels are dist'd $0 \rightarrow \infty$

$$E_K = \frac{\hbar^2}{2m}\left(K_x^2 + K_y^2 + K_z^2\right)$$



$K_{x,y,z} = \frac{2n\pi}{L}$, $n = 0, \pm 1, \pm 2, \ldots$

(cube L)

$$\psi_{\vec{k}}(\vec{r}) = e^{j(\vec{k}\cdot\vec{r})} \Rightarrow \text{travelling waves}$$

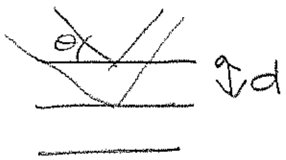
w/ $\vec{p} = \hbar\vec{k}$

Now consider effect of pdic ion cores

$\Rightarrow$ e^- weakly perturbed by the core

$\Rightarrow$ nearly free e^- model $\Rightarrow$ metals

<u>Bragg</u>



$2d\sin\theta = n\lambda$

Bragg reflect of e^- waves in xtls $\rightarrow$ energy gaps

simple lattice, w/ constant a.

Bragg cond'n of wave: $k = \pm\frac{n\pi}{a}$ $n = 1, 2, \ldots$ (1D)

$\therefore$ band gaps occur at

$$K = \pm\frac{n\pi}{a}$$

$$K = \pm \frac{\pi}{a}$$

$\psi(\pm \frac{\pi}{a})$ are not travelling waves

$\underbrace{e^{j\pi x/a} \text{ or } e^{-j\pi x/a}}$ (like free e^-)

$\psi(k)$ is composed of equal parts of right travelling + left travelling waves $\Longrightarrow$ standing wave

$$\underbrace{e^{\pm j\pi x/a}}_{\text{travelling}} = \cos\left(\frac{\pi x}{a}\right) \pm j\sin\left(\frac{\pi x}{a}\right)$$

$$\text{standing}\begin{cases} \psi(+) = e^{j\pi x/a} + e^{-j\pi x/a} = 2\cos\left(\frac{\pi x}{a}\right) \\ \psi(-) = e^{j\pi x/a} - e^{-j\pi x/a} = j2\sin\left(\frac{\pi x}{a}\right) \end{cases}$$

these waves "pile up" e^- in different

$\psi(+)$ + $\psi(-)$ have diff. values of P.E. in vicinity of ion cores

$\Longrightarrow$ gaps

$$\rho = \psi^*\psi = |\psi|^2$$

pure travelling: $\psi^*\psi = e^{j\pi x/a} e^{-j\pi x/a} = 1$

but for $\psi(+)$: $\rho(+) = |\psi(+)|^2 \propto \cos^2 \frac{\pi x}{a}$

e^- pile up @ ion centers

for $\psi(-)$: $\rho(-) \propto \sin^2\left(\frac{\pi x}{a}\right)$

e^- pile up away from centers

More on band gap

TISE (1D)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

pdic pot'l $\quad V(x) = V(x+a)$

pd $= a$

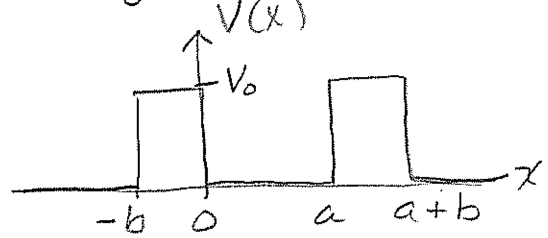
$\psi(x) = e^{jkx}\underbrace{u(x)}_{\text{pd. } a}$ ← Bloch wavefn

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx}\left[e^{jkx}u(x)\right] + V(x)e^{jkx}u(x) = Ee^{jkx}u(x)$$

$$-\frac{\hbar^2}{2m}\left[-k^2u(x) + 2jk\frac{du}{dx} + \frac{d^2u}{dx}\right]\cancel{e^{jkx}} + V(x)\cancel{e^{jkx}}u(x) = E\cancel{e^{jkx}}u(x)$$

$$= \frac{\hbar^2}{2m}\left(\frac{1}{j}\frac{d}{dx} + k\right)^2 u(x) + V(x)u(x) = Eu(x)$$

Now given



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$0 < x < a$: $V(x) = 0$

$\Rightarrow \psi(x) = Ae^{jKx} + Be^{-jKx} \qquad E = \frac{\hbar^2K^2}{2m}$

$-b < x < 0$: $V(x) = V_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \overbrace{V_0\psi = E\psi}$$

$$\Rightarrow \psi(x) = Ce^{Qx} + De^{-Qx}$$

$$V_0 - E = \frac{\hbar^2 Q^2}{2m}$$

$a < x < a+b$

$$\Rightarrow \psi(x) = \psi(-b < x < 0)\, e^{jk(a+b)}$$

$$\psi(0):\ Ae^{jK(0)} + Be^{-jK(0)} = Ce^{Q(0)} + De^{-Q(0)}$$

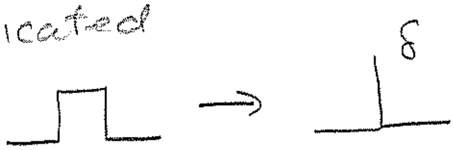
$$A + B = C + D$$

contin in $\frac{d\psi}{dx}$

$$\left.\frac{d\psi}{dx}\right|_{x=0} \Rightarrow jK(A-B) = Q(C-D)$$

repeat @ $x=a \Rightarrow$ 4 eqns, 4 unk.

complicated

let 

$b \to 0,\ V_0 \to \infty$

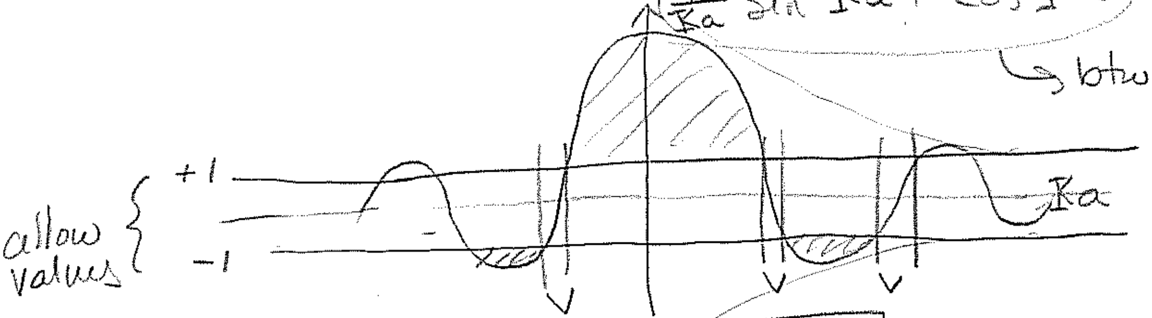
$$\left(\frac{P}{Ka}\right)\sin Ka + \cos Ka = \cos ka$$

$$P = \frac{Q^2 ba}{2}$$ Kronig Penny

Ex: $P = \frac{3\pi}{2}$

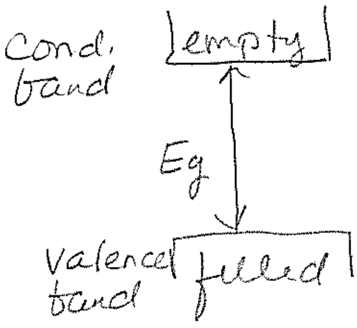
$$\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka$$

btwn -1 & 1

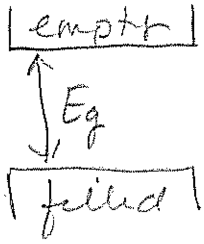


$$Ka = \sqrt{\frac{2mE}{\hbar^2}}\, a$$

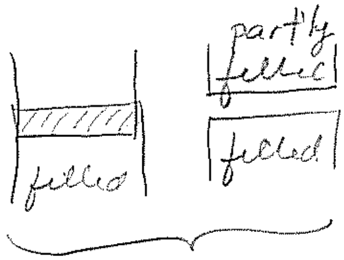
Typical band structure @ 0K



insulator

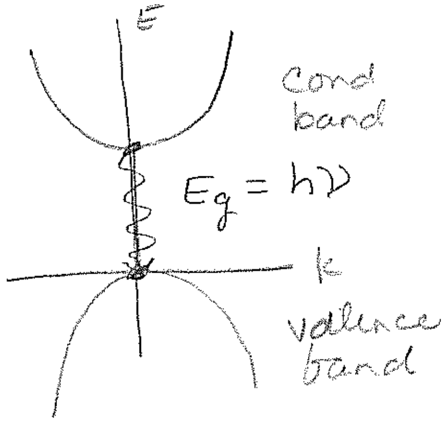


s/c



metals
conductors

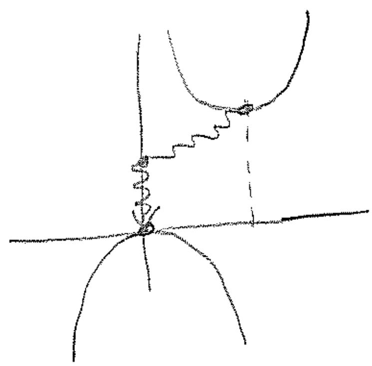
E vs. $\vec{k}$



$\Rightarrow$ Direct GaAs

$h\nu \Rightarrow$ visible $\Rightarrow$ LED

red $\leftrightarrow$ 1.9eV



$\Rightarrow$ Indirect Si

$\rightarrow$ change in E

change in k

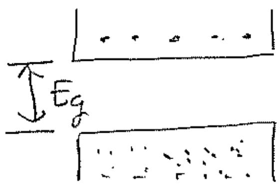
$\Rightarrow$ momentum

Charge carriers

metal – e^- move easily in E-field

s/c – e^- move to cond. band, leave "hole" in valence band (empty state)

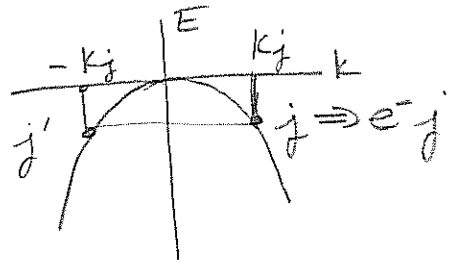
$\Rightarrow$ e^--hole pairs



Si ~ $10^{10}\ \frac{\text{pairs}}{\text{cm}^3}$

$10^{22}\ \frac{\text{atom}}{\text{cm}^3}$

Full valence band



@ 0K

e^-_j w/ v_j

then $e^-_{j'}$ w/ $-v_j$

current density

$N\ \frac{e^-}{\text{cm}^3}$

$$J = \boxed{-q \sum_{i=1}^{N} v_i = 0}$$

Now add thermal energy

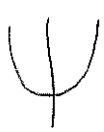
excites j^{th} e^- $\Rightarrow$ leaves.

$\Rightarrow$ unbalanced velocities

$$J = \underbrace{\cancel{-q \sum_{i=1}^{N} v_i}}_{0} - (-q)v_j = +\underline{q}\, v_j$$

holes act like + charge carrier

(actually unbalanced e^- $(-q)(-v_j)$)

e^- E  hole E 

Band diagrams

$(E, \vec{k}) \Rightarrow$ total E $(PE + KE)$ vs. $\vec{k}$

$\vec{k} \propto \vec{p} \propto \vec{v}$

$k = 0 \Rightarrow v = 0 \Rightarrow KE = 0 \rightarrow$ only PE

Effective mass

e^- not completely free

$\Rightarrow$ analysis needs to use an altered mass to acct for E band shape.

$$KE = \frac{1}{2} m v^2 = \frac{1}{2} \frac{p^2}{m} = \frac{\hbar^2 k^2}{2m}$$

$\underbrace{e^- \text{ mass}}_{\text{effective}}$ inv. related to curvature $\downarrow$ $\frac{d^2E}{dk^2}$

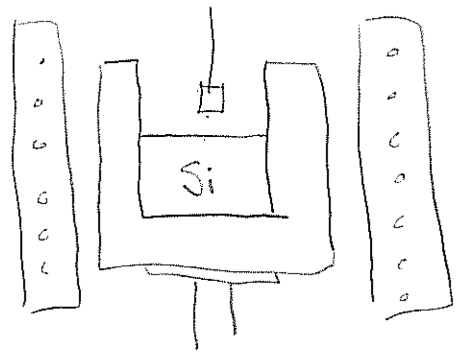
$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*} \rightarrow \text{effective mass}$$

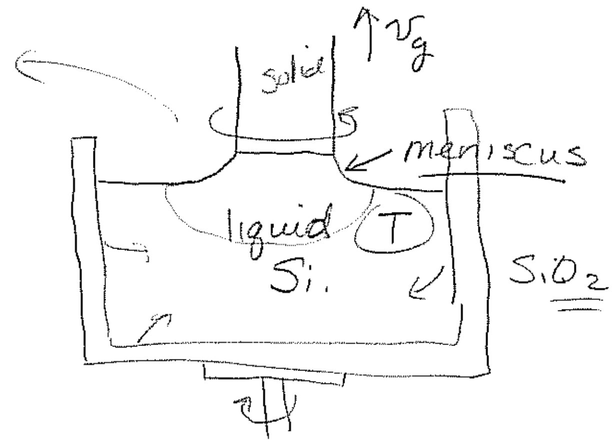
$$\boxed{m^* = \frac{\hbar^2}{d^2E/dk^2}}$$

Intrinsic + Extrinsic Mat'ls

intrinsic - no impurities or lattice defects

Czochralski





intrinsic

e^-/hole pairs → only charge carriers

↳ $n \frac{e^-}{cm^3} = p \frac{holes}{cm^3} = n_i$: intrinsic carrier concentration

e^-/hole generation + recomb'n ⇒ equal

$r_i = g_i$ → rates

these are fn of equilibrium concentration thus of T

$$r_i = \alpha n_o p_o = \alpha n_i^2 = g_i$$

extrinsic - purposely introduce impurities ⇒ doping

n-type → mostly e^-

p-type → mostly holes.

- introduces energy levels into band structure

↳ energy level close to cond. or val band

donor ↲ ↳ acceptor

5^{th} e^-, loosely bound

$$nE = \frac{mq^4}{2K^2\hbar^2}$$

$$K = 4\pi\epsilon_0\epsilon_r$$