Solid State Physics 2012

(1) Lennard Jones Potential

$$U(R) = 4\varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right]$$

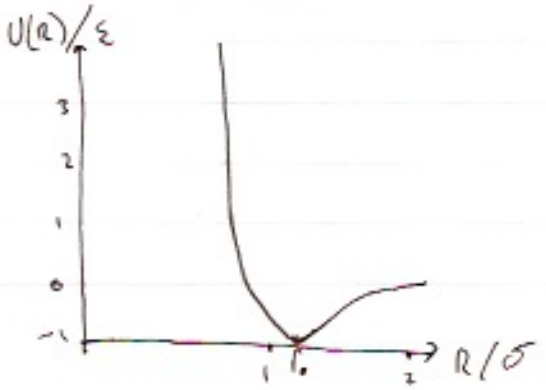
equilibrium when $\frac{dU}{dR} = 0$

$$\Rightarrow \quad U(R) = \frac{4\varepsilon\sigma^{12}}{R^{12}} - \frac{4\varepsilon\sigma^{6}}{R^{6}} \qquad \left.\frac{dU}{dR}\right|_{R=R_0} = 0 = \frac{-48\sigma^{12}}{R^{13}} + \frac{24\sigma^{6}}{R^{7}}$$

$$-\frac{2\sigma^{12}}{R^{13}} + \frac{\sigma^{6}}{R^{7}} = 0$$

$$-2\sigma^{6} + R^{6} = 0$$

$$\boxed{R = \sqrt[6]{2}\,\sigma}$$



(2) Intrinsic semiconductor means $n_i = p_i$

$$\Rightarrow \quad A\,(m_e^* T)^{3/2} e^{(\mu - E_g)/kT} = A(m_h^* T)^{3/2} e^{-\mu/kT}$$

$$m_e^{*\,3/2} e^{(\mu - E_g)/kT} = m_h^{*\,3/2} e^{-\mu/kT}$$

$$m_e^{*\,3/2} e^{(2\mu - E_g)/kT} = m_h^{*\,3/2}$$

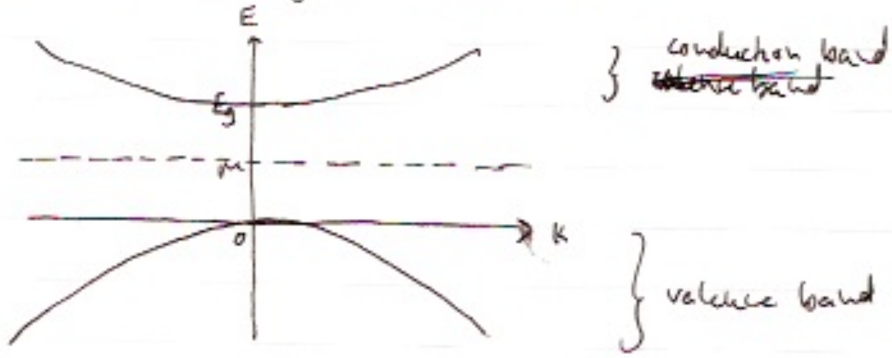
$$e^{(2\mu - E_g)/kT} = \left(m_h^*/m_e^*\right)^{3/2}$$

$$\frac{2\mu - E_g}{kT} = \ln\left(\frac{m_h^*}{m_e^*}\right)^{3/2}$$

$$2\mu = E_g + \tfrac{3}{2}kT\ln\left(m_h^*/m_e^*\right)$$

$$\mu = \tfrac{1}{2}E_g + \tfrac{3}{4}kT\ln\left(m_h^*/m_e^*\right)$$

Therefore for a typical semiconductor:

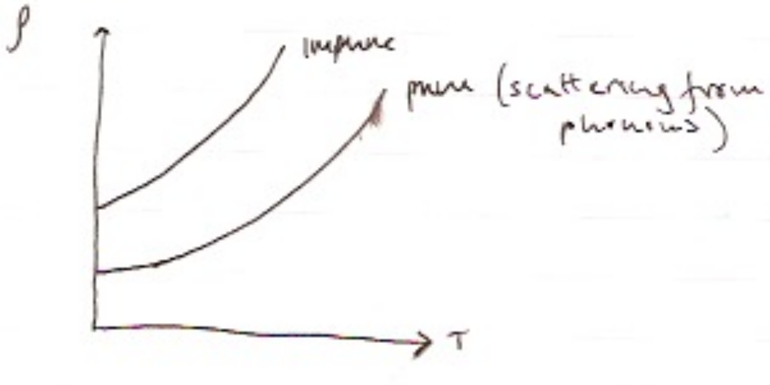


(3) We know that

$$\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$$

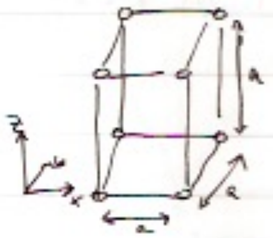
from Mattheisen's rule $\rho = \rho_0 + \rho_{phonon}(T)$

therefore:

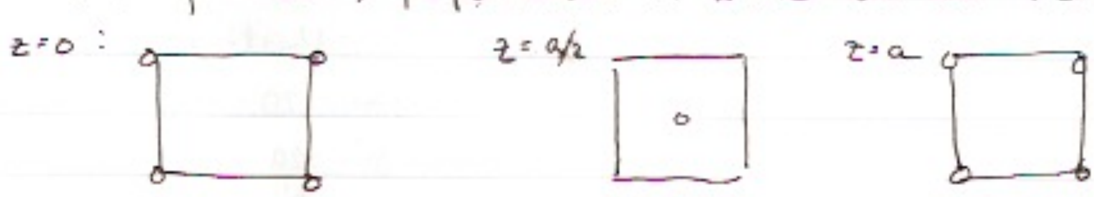


$$\frac{1}{\tau} = \frac{1}{\tau_i} + \frac{1}{\tau_p}$$

(4) Conventional 3D unit cell for simple cubic



And so for BCC, perpendicular to [0,0,1] direction, cross section



Max packing fraction achieved if all atoms were touching in unit cell

PF = No of atoms in unit cell × $\frac{\text{volume of 1 atom}}{\text{vol of unit cell}}$

vol of unit cell = a^3

No of atoms = 2 (corner atoms contribute 1/8)

vol of atom = $\frac{1}{3} 4\pi r^3$

$\sqrt{3a^2} = 4r \Rightarrow \sqrt{3}a = 4r \Rightarrow a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3$

$\Rightarrow PF = \frac{2 \times 4\pi \cancel{r^3}}{3 \times \frac{64}{3\sqrt{3}} \cancel{r^3}} = \frac{24\sqrt{3}\pi}{192} \sim 68\%$

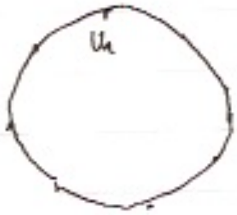
(5)

N atoms

Length $L = aN$

Apply periodic boundary conditions:

Still N atoms



Position/displacement of n^{th} atom in chain is

$U_n = e^{ikna}$

but $U_n = U_{n+N} = e^{ika(n+N)}$

$\Rightarrow kNa = 2\pi \times \text{integer}$

$\Rightarrow \Delta k = \frac{2\pi}{Na} = \frac{2\pi}{L}$

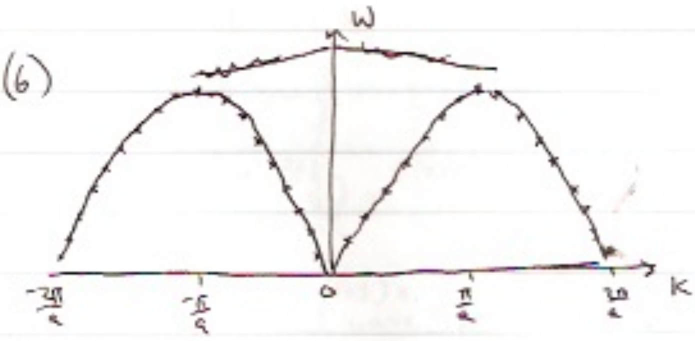
Brillouin Zone Boundary at $k = \pm \pi/a$

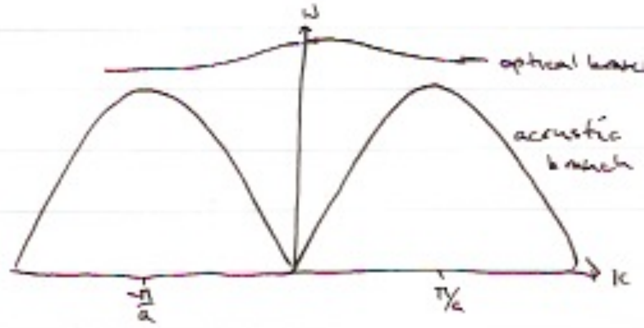
$\Rightarrow$ # of modes in BZB = Spin Degeneracy $\times$ $\frac{\text{Length of Brillouin Zone}}{\text{spacing between modes}}$

$$\#\text{ of modes} = \underset{\text{spin up + down.}}{2} \times \frac{\delta k}{\Delta k} = 2 \times \frac{(\pi/a)}{(2\pi/Na)} = 2N$$

If the electron lies with its wavevector on Brillouin Zone Boundary, it has the highest possible angular frequency ω of oscillation. If it surpasses $k = \pi/a$, the frequency drops and the electron reverses direction (Umklapp)

(6)





(7) (a) $F = \sum_j f_j e^{i\underline{Q}\cdot\underline{r}_j}$

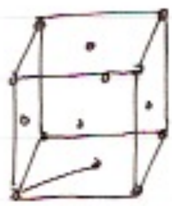
f_j - scattering strength

$\underline{Q} = \underline{k} - \underline{k}'$ change in wavevector

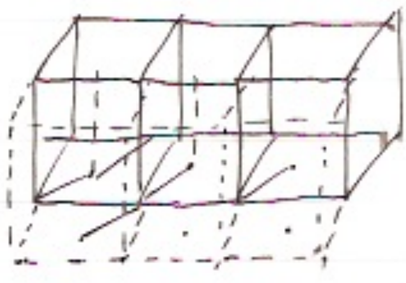
$\underline{r}_j$ - position of atom in cell

(b) $\underline{Q} = \underline{G}$ where $\underline{G}$ is reciprocal lattice vector

(c) An FCC looks like



This can be decomposed into a simple cubic lattice and a basis of one atom since it is uniform everywhere throughout the lattice so consider simple cubic at $(0,0,0)$ and the basis $(\frac{a}{2}, \frac{a}{2}, 0)$ being chosen



could just as easily define a simple cubic at $(\frac{a}{2}, \frac{a}{2}, 0)$ plus a basis at $(a, a, 0)$

The coordinates of the basis is $(0,0,0)$

The other coordinates are $(\frac{a}{2}, \frac{a}{2}, 0)$, $(0, \frac{a}{2}, \frac{a}{2})$, $(\frac{a}{2}, 0, \frac{a}{2}$

(d) $$F = \sum_j f_j e^{i Q \cdot r_j}$$

$$F = f_j e^{i\frac{2\pi}{a}(h,k,l)\cdot\frac{a}{2}(0,0,0)} + f_j e^{i\frac{2\pi}{a}(h,k,l)\cdot(1,1,0)\frac{a}{2}} + f_j e^{i\frac{2\pi}{a}(h,k,l)\cdot(1,0,1)\frac{a}{2}} + f_j e^{i\frac{2\pi}{a}(h,k,l)\cdot(0,1,1)\frac{a}{2}}$$

$$F = f_j + f_j e^{i\pi(h+k)} + f_j e^{i\pi(h+l)} + f_j e^{i\pi(k+l)}$$

$$F = \begin{cases} 4f & \text{if } h,k,l \text{ all even or odd} \\ 0 & \text{if mixture of odd/even} \end{cases}$$

(e)

2θ	$\sin\theta$	$\sin^2\theta$	$\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$\frac{\sin^2\theta}{2\times\sin^2\theta_{min}}$	$\frac{\sin^2\theta}{3\times\sin^2\theta_{min}}$	N
37.42	0.32	0.10	1	2	3	3 : (1,1,1)
43.48	0.37	0.14	1.4	2.8	4.2	4 : (2,0,0)
63.17	0.52	0.27	2.7	5.4	8.1	8 : (2,2,0)

$\Rightarrow$ FCC

use Bragg's law $\lambda = 2d\sin\theta$

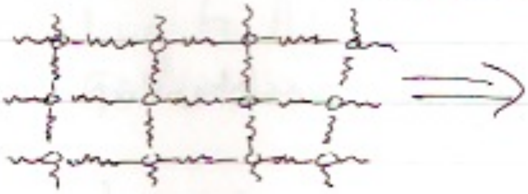
$$d = \frac{a}{\sqrt{N}}$$

$$\Rightarrow \lambda = \frac{2a\sin\theta}{\sqrt{N}} \Rightarrow \frac{\sqrt{N}\lambda}{2\sin\theta} = a$$

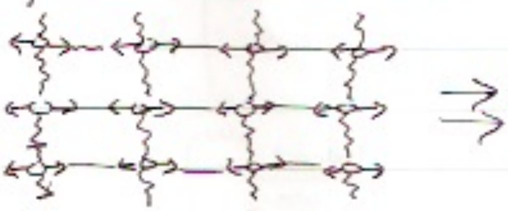
$\sin\theta$	N	a
0.32	3	4.06 Å
0.37	4	4.05 Å
0.52	8	4.08 Å

$$\langle a\rangle = \frac{1}{3}(4.06 + 4.08 + 4.05) = 4.06\,\text{Å}$$

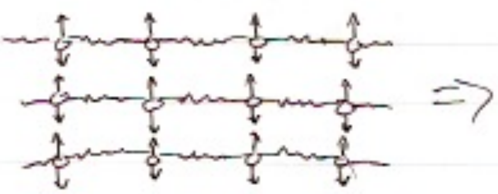
(8) (a) A 2D solid like the mentioned one looks like



Longitudinal waves look like



transverse waves



(b) $C_V = \frac{dU}{dT} = Nk_B \times f$ where f is the number of degrees of freedom?

According to Einstein

$$U = f N k_B \Theta_E \left(\frac{1}{2} + \frac{1}{e^{\Theta_E/T} - 1} \right) \qquad f = 2 \text{ for 2D}$$

$$\Rightarrow C_V = \frac{dU}{dT} = 2Nk_B.$$

(c) Assumptions of Debye Theory

- dispersionless relation (linear) relationship between ω and k $\quad \omega/k = d\omega/dk = V_s$
- crystals are harmonic and have normal modes of oscillation
- crystals are isotropic

(d)

$$g(k)\,dk = g(\omega)\,d\omega$$

$$g(k)\,dk = \frac{2\pi k}{(2\pi/L)^2}\,dk = g(\omega)\,d\omega$$

$$g(\omega) = \frac{2\pi k L^2}{4\pi^2}\frac{dk}{d\omega} = \frac{kL^2}{2\pi V_s} = \frac{\omega L^2}{2\pi V_s^2}$$

$$N = \int_0^{\omega_0} \frac{\omega L^2}{2\pi V_s^2}\,d\omega = \frac{\omega_0^2 L^2}{4\pi V_s^2}$$

but $\quad \dfrac{L^2}{2\pi V_s^2} = \dfrac{g(\omega)}{\omega}$

$$\Rightarrow \quad N = \frac{\omega_0^2\, g(\omega)}{2\omega}$$

$$\frac{2N\omega}{\omega_0^2} = g(\omega) \qquad \text{QED}$$

(e) According to Debye Theory

$$E = U = U_z + 2\int_0^\infty \hbar\omega\, n(\omega)\, g(\omega)\, d\omega$$

and zero point energy $U_z \to 0$

$$U = 2\int_0^\infty \hbar\omega\, n(\omega)\, g(\omega)\, d\omega$$

$$U = 2\int_0^{\omega_D} \frac{\hbar\omega}{e^{\hbar\omega/kT}-1} \times \frac{2N\omega}{\omega_D^2}\, d\omega$$

$$U = \frac{4N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar\omega^2}{e^{\hbar\omega/kT}-1}\, d\omega \qquad \underline{\text{QED}}$$

(f)

$$C_v = \frac{dU}{dT} = \frac{4N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar\omega^2}{-(e^{\hbar\omega/kT}-1)^2} \times -e^{\hbar\omega/kT} \times \frac{\hbar\omega}{kT^2}\, d\omega$$

$$C_v = \frac{4N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar^2\omega^3}{kT^2}\, \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT}-1)^2}\, d\omega$$

subs $\frac{\hbar\omega}{kT} = x \qquad \frac{dx}{d\omega} = \frac{\hbar}{kT} \qquad d\omega = dx\,\frac{kT}{\hbar}$

$$C_v = \frac{4N}{\omega_D^2}\int_0^\infty \frac{\hbar^{\cancel{2}}\omega^3}{kT^{\cancel{2}}}\, \frac{e^x}{(e^x-1)^2}\, \frac{\cancel{kT}}{\cancel{\hbar}}\, dx = \frac{4N}{\omega_D^2}\int_0^\infty \frac{\hbar\omega^3}{T}\, \frac{e^x}{(e^x-1)^2}\, dx$$

$$x^3 = \frac{\omega^3\hbar^3}{k^3T^3} \qquad \omega^3 = \frac{x^3k^3T^3}{\hbar^3}$$

$$C_v = \frac{4N}{\omega_D^2}\int_0^\infty \frac{k^3T^2}{\hbar^3}\, \frac{x^3e^x}{(e^x-1)^2}\, dx \qquad \Theta_D = \frac{\hbar\omega_D}{k_B} \qquad \frac{1}{\omega_D^2} = \frac{\hbar^2}{k_B^2\Theta_D^2}$$

$$C_v = \frac{4N\cancel{k^2}T^2k^{3}}{\cancel{k^2}\cancel{\hbar^2}\Theta_D^2}\int_0^\infty \frac{x^3e^x}{(e^x-1)^2}\, dx = 4Nk\left(\frac{T}{\Theta_D}\right)^2 \times 7.21 = 28.8Nk\left(\frac{T}{\Theta_D}\right)^2$$

(9) (a) Main assumptions of free electron model:

- valence electrons can be treated as free electrons travelling under constant potential
- electrons are non interacting.

(b) Free model is successful in explaining

- electrical + thermal conductivity
- temp dependence of specific heat

failures of free electron model:

- some specific heat calculations are overestimated compared to experimental result
- fails to describe quantum phenomena and blackbody radiation e.g. photoelectric effect and compton scattering

(c)

$$g(\varepsilon) = 2 \times \frac{4\pi k^2}{\left(\frac{2\pi}{L}\right)^3} \frac{dk}{dE} = 2 \times \frac{Vk^2}{2\pi^2} \frac{dk}{dE} = \frac{Vk^2}{\pi^2} \frac{dk}{dE}$$

but $E = \frac{\hbar^2 k^2}{2m}$ $\quad \frac{dE}{dk} = \frac{2k\hbar^2}{2m} = \frac{k\hbar^2}{m}$

$$\cancel{\frac{\hbar^2}{2m} = \frac{E}{k^2}} \qquad \cancel{\frac{dE}{dk} = \frac{2E}{k}} \qquad E = \frac{dE}{dk}\frac{k}{2}$$

$$\cancel{g(E) = \frac{Vk^2}{\pi^2} \frac{m}{k\hbar^2}}$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$k = \left(\frac{2m}{\hbar^2}\right)^{1/2} E^{1/2}$$

$$g(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$$

(d) $$N = \int_0^{E_f} g(E)\,dE$$

$$N = \int_0^{E_f} \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}\,d\varepsilon$$

$$N = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\frac{2}{3}\varepsilon^{3/2}\right]_0^{E_f}$$

$$N = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}E_f^{3/2}$$

$$\left(\frac{3N\pi^2}{V}\right)^{2/3} = \frac{2m}{\hbar^2}E_f$$

$$E_f = \frac{\hbar^2}{2m}\left(\frac{3N\pi^2}{V}\right)^{2/3}$$

(e) $$E_f^k = \frac{\left(\frac{6.63\times10^{-34}}{2\pi}\right)^2}{2\times9.11\times10^{-31}}\left(\frac{12\pi^2}{(5.23\times10^{-10})^3}\right)^{2/3}$$

$$E_f^k = 5.388\times10^{-19}\text{ J} = 3.37\text{ eV}.$$

$$p_f = \sqrt{2mE_f}$$

$$v_f = p_f/m = \frac{\sqrt{2\times9.11\times10^{-31}\times5.388\times10^{-19}}}{9.11\times10^{-31}} = 1.09\times10^6\text{ ms}^{-1}.$$

Fermi Velocity is high, but around what is expected by Free Electron Model

(f) $|k_f| = \left| \frac{\sqrt{2mE_f}}{\hbar} \right| = \cancel{\ldots}$

$k_f = \frac{1}{\hbar}\left(\frac{2m\hbar^2}{2m}\left(\frac{3N\pi^2}{V}\right)^{2/3}\right)^{1/2}$

$k_f = \frac{\hbar}{\hbar}\left(\frac{3N\pi^2}{V}\right)^{1/3} = \left(\frac{3N\pi^2}{V}\right)^{1/3}$

vol of fermi surface is $\frac{4}{3}\pi k_f^3 = V_{fs}$

$V_{fs} = \frac{4}{\cancel{3}}\pi \frac{\cancel{3}N\pi^2}{V} = \frac{4N\pi^3}{V}$ $\quad V = a^3$ and monovalent $\Rightarrow N = 1$

$$\boxed{V_{fs} = \frac{4\pi^3}{a^3}}$$

Vol of 1st BZ $= V_{BZ} = \left(2\pi/a\right)^3 = 8\pi^3/a^3$

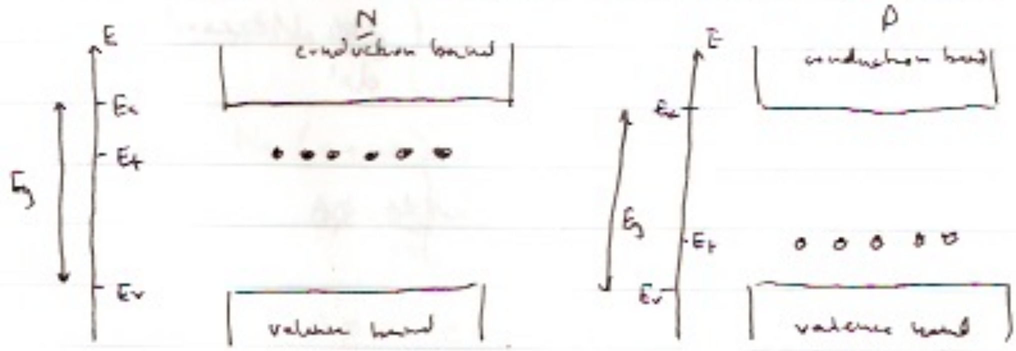
$$\frac{Vol_{fs}}{Vol_{BZ}} = \frac{4\pi^3/a^3}{8\pi^3/a^3} = \frac{1}{2}$$

If valency increased to 2, $V_{fs}^{2val} = V_{fs}^{1val} \times 2$

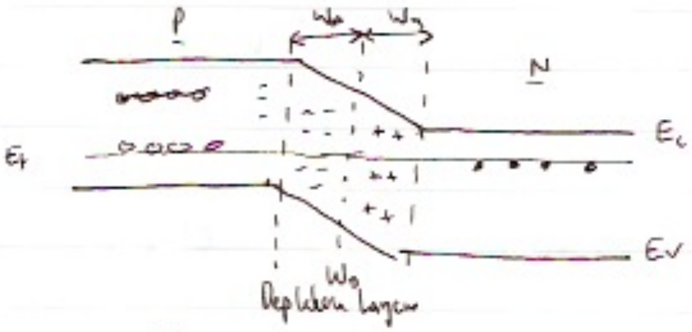
it would become twice as big

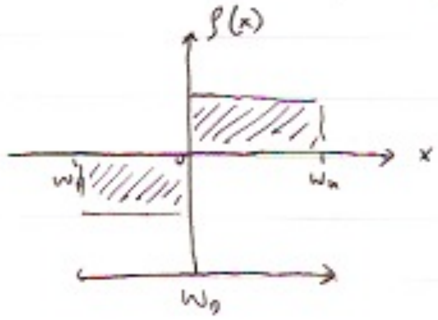
(10) (a) P type semiconductor has excess holes

N type semiconductors has excess electrons

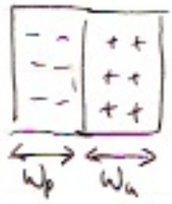


(b) At a P-N junction, fermi energies are equal:





(c) In the depletion layer:



$$-\frac{\rho(x)}{\varepsilon_0\varepsilon_r} = \int \frac{d^2\phi}{dx^2}$$ according to Poisson's Eq

$$\int \mathcal{E}dx = -\int \frac{d\phi}{dx} = 0$$

in Wp region $W_p \le \cancel{x} < 0$:

$$-\frac{eN_A W_p}{\varepsilon_0\varepsilon_r} + k = 0 \quad \Rightarrow \quad k = \frac{eN_A W_p}{\varepsilon_0\varepsilon_r} \quad (1)$$

in Wn region $0 < x \le W_n$

$$\frac{eN_D W_p}{\varepsilon_0\varepsilon_r} + k = 0 \quad \Rightarrow \quad k = \frac{-eN_D W_n}{\varepsilon_0\varepsilon_r} \quad (2)$$

$$(1)\ \Big|\ \frac{\partial\phi}{\partial x} = \frac{eN_a(W_p + x)}{\varepsilon_0\varepsilon_r} \ (A) \qquad (2)\ \Big|\ \frac{\partial\phi}{\partial x} = \frac{eN_D(x - W_n)}{\varepsilon_0\varepsilon_r} \ (B)$$

We want a continuous field

$$\frac{eN_a(x + W_p)}{\varepsilon_0\varepsilon_r} = \frac{eN_D(x - W_n)}{\varepsilon_0\varepsilon_r}$$

$$\frac{eN_A W_p}{\cancel{\varepsilon_0\varepsilon_r}} = -eN_D W_n$$

Integrating

$$(A)\ \phi = \frac{eN_A(W_p + x)^2}{2\varepsilon_0\varepsilon_r} + k_1 \qquad (B)\ \phi = k_2 - \frac{eN_D(x - W_n)^2}{2\varepsilon_0\varepsilon_r}$$

$$k_1 + k_2 = \Delta\phi_0$$

choose $k_1 = 0 \quad \therefore k_2 = \Delta\phi_0$

$$\Rightarrow \phi = \frac{eN_a(x + W_p)^2}{2\varepsilon_0\varepsilon_r} \qquad \phi = \Delta\phi_0 - \frac{eN_D(x - W_n)^2}{2\varepsilon_0\varepsilon_r}$$

(d) Neutrality of junction given by

$$-eN_A w_p = eN_D w_n$$

$$\frac{1}{2\varepsilon_0\varepsilon_r} eN_A (x+w_p)^2 = \Delta\phi - eN_D (x-w_n)^2 \frac{1}{2\varepsilon_0\varepsilon_r}$$

$$\Delta\phi = \frac{eN_A(x+w_p)^2 + eN_D(x-w_n)^2}{2\varepsilon_0\varepsilon_r}$$

$$\Delta\phi = \frac{e\left(N_A w_p^2 - N_D w_n^2\right)}{2\varepsilon_0\varepsilon_r} \quad \text{as } x \to 0$$

$$w_p = \frac{N_D w_n}{N_A}$$

$$\frac{2\varepsilon_0\varepsilon_r \Delta\phi}{e} = N_A \left(\frac{N_D w_n}{N_A}\right)^2 + N_D w_n$$

$$\frac{2\varepsilon_0\varepsilon_r \Delta\phi}{e} = \frac{N_D^2 w_n^2}{N_A} + N_D w_n^2$$

$$\frac{2\varepsilon_0\varepsilon_r \Delta\phi}{e} = w_n^2 \left(\frac{N_D^2}{N_A} + N_D\right)$$

$$\frac{2\varepsilon_0\varepsilon_r \Delta\phi}{e} = w_n^2 \left(\frac{N_D^2 + N_A N_D}{N_A}\right)$$

$$\frac{2\varepsilon_0\varepsilon_r \Delta\phi}{e} = w_n^2 \left(\frac{N_D}{N_A}(N_D + N_A)\right)$$

$$w_n = \left[\frac{2N_A\varepsilon_0\varepsilon_r\Delta\phi}{N_D e (N_D + N_A)}\right]^{1/2} \qquad \underline{\text{QED}}.$$

$$w_p = \frac{N_D}{N_A}\left[\frac{2N_A\varepsilon_0\varepsilon_r\Delta\phi}{eN_D(N_D+N_A)}\right]^{1/2} = \left[\frac{2N_D\varepsilon_0\varepsilon_r\Delta\phi}{eN_A(N_A+N_D)}\right]^{1/2}$$