University of Michigan – Shanghai Jiao Tong University Joint Institute
Center of Optics and Optoelectronics

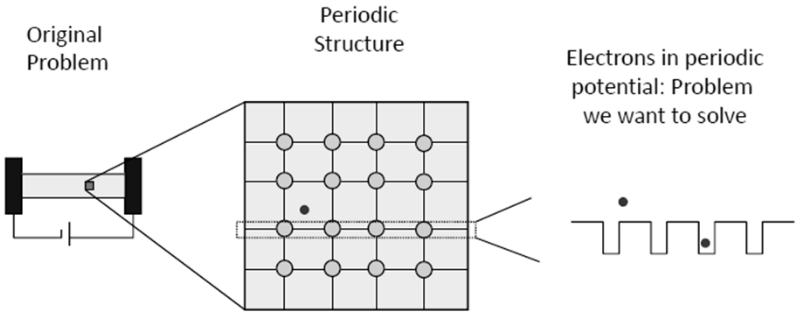
VE 320 – Summer 2012
Introduction to Semiconductor Device

Instructor: Professor Hua Bao

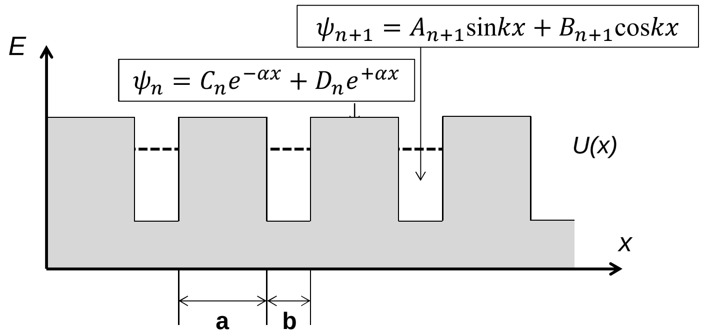
Previous Lecture

- In order to understand the transport property of semiconductor, we need to understand the chemical composition and atomic arrangements.
- Crystalline structure can be built by repeating basic building blocks… Bravais lattice, basis
- Diamond and zinc-blende structure
- To identify crystal planes…Miller Indices, vector indices

Getting back to Crystals



Finally (almost) a Real Problem



$$p = a + b$$

But N atoms have 4N unknowns constants to find…

For large N, is there a better way?

Five Steps to Solve this Problem

1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

2) $$\psi(x=-\infty)=0$$ $$\psi(x=+\infty)=0$$

3) $$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$ $$\frac{d\psi}{dx}\bigg|_{x=x_B^-} = \frac{d\psi}{dx}\bigg|_{x=x_B^+}$$

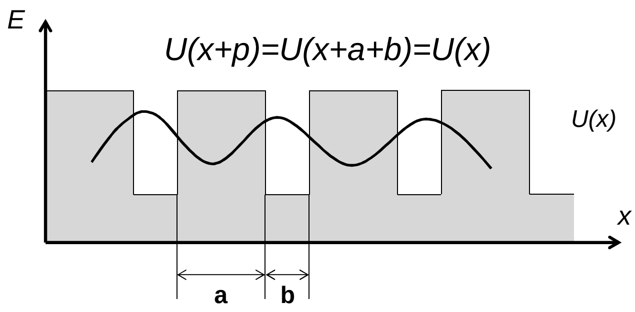
4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

- N is very large for crystal, but changing steps 2 and 3 a little bit we can still solve the problem in a few minutes!

Periodic U(x) and Bloch Theorem

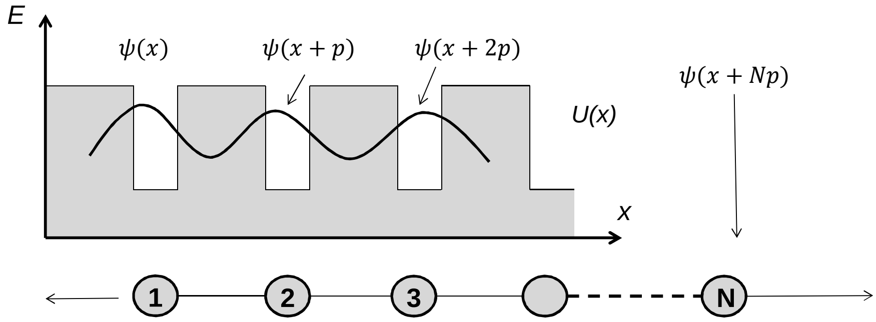
not our old (k)

$$|\psi(x)|^2 = |\psi(x+p)|^2 \Longrightarrow \psi(x+p) = \psi(x)\,e^{ikp}$$



$$p = a + b$$

Phase Factor for N Cells

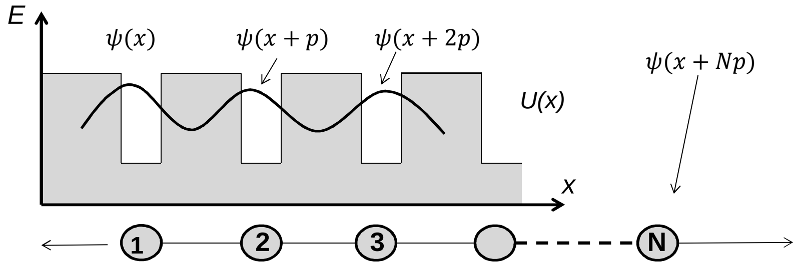


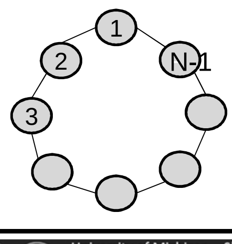
$$\psi(x+p) = \psi(x)e^{ikp}$$

$$\psi(x+2p) = \psi(x)e^{2ikp}$$

$$\psi(x+Np) = \psi(x)e^{Nikp}$$

Step 2: Periodic Boundary Condition





$$\psi(x+Np) = \psi(x)e^{Nikp} = \psi(x)$$

$$e^{Nikp} = 1 = e^{\pm 2\pi n i}$$

$$k = \pm\frac{2\pi n}{Np} \qquad n = -\frac{N}{2}, \ldots -1,0,1, \ldots, \frac{N}{2}$$

$$k_{max} = \frac{\pi}{p}, k_{min} = -\frac{\pi}{p}$$

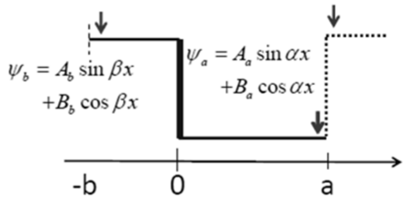
Step 3: Boundary Conditions

$$\psi\big|_{x=0^-} = \psi\big|_{x=0^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^-} = \left.\frac{d\psi}{dx}\right|_{x=0^+}$$

$$B_a = B_b$$
$$\alpha A_a = \beta A_b$$

$$\alpha \equiv \sqrt{2mE/\hbar^2} \qquad \beta \equiv i\sqrt{2m(U_0 - E)/\hbar^2}$$



$$\psi_a\big|_{x=a} = \psi_b\big|_{x=-b}\, e^{ikp}$$

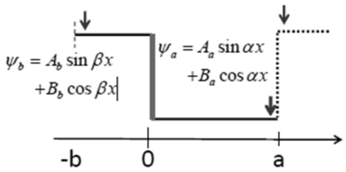
$$\left.\frac{d\psi_a}{dx}\right|_{x=a} = \left.\frac{d\psi_b}{dx}\right|_{x=-b} e^{ikp}$$

$$A_a \sin\alpha a + B_a \cos\alpha a =$$
$$e^{ik(a+b)}[-A_b \sin\beta b + B_b \cos\beta b]$$

$$\alpha A_a \sin\alpha a - \alpha B_a \cos\alpha a =$$
$$e^{ik(a+b)}[\beta A_b \sin\beta b + \beta B_b \cos\beta b]$$

Step 4: Det(matrix)=0 for Energy Levels

$$B_a = B_b$$
$$\alpha A_a = \beta A_b$$



$$A_a \sin\alpha a + B_a \cos\alpha a =$$
$$e^{ik(a+b)}[-A_b \sin\beta b + B_b \cos\beta b]$$

$$\alpha A_a \sin\alpha a - \alpha B_a \cos\alpha a =$$
$$e^{ik(a+b)}[\beta A_b \sin\beta b + \beta B_b \cos\beta b]$$

$$\Rightarrow \begin{pmatrix} 0 & 1 & 0 & -1 \\ \alpha & 0 & \beta & 0 \\ * & * & & \\ * & & & \end{pmatrix} \begin{bmatrix} A_a \\ B_a \\ A_b \\ B_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

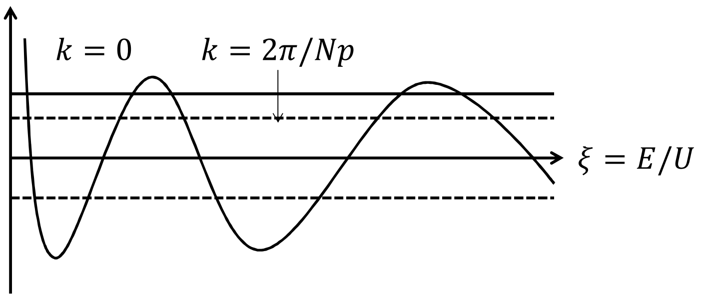
$$\Downarrow$$

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \text{...........} = \cos kp \qquad \xi \equiv \frac{E}{U_0} \quad \alpha_0 \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

Graphical Solution to Energy Levels

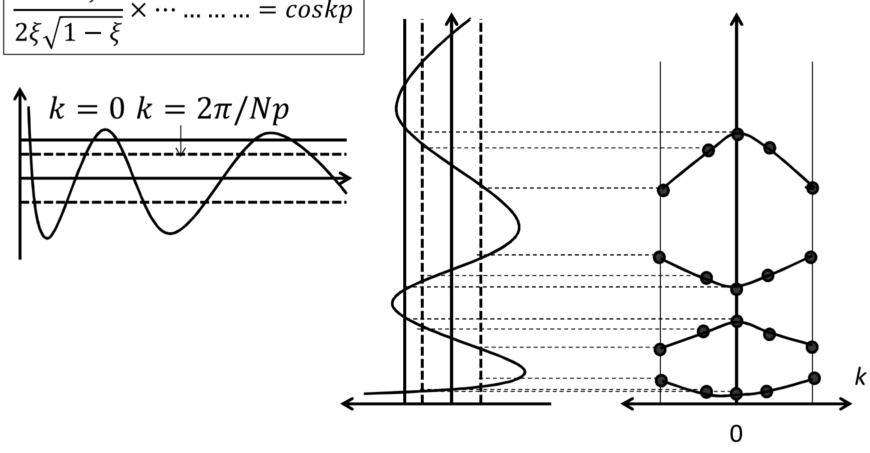
$$\frac{1-\xi}{2\xi\sqrt{1-\xi}} \times \cdots \dots \dots \dots = coskp$$

$$k = \pm\frac{2\pi n}{Np} \quad n = -\frac{N}{2}, \dots - 1,0,1, \dots, \frac{N}{2}$$

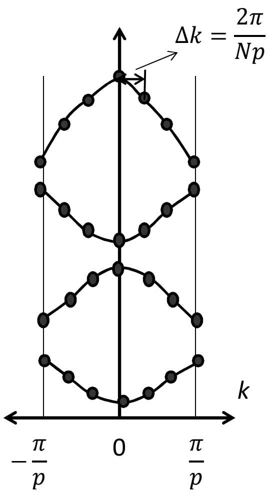


Energy Band Diagram

$$\frac{1-\zeta}{2\xi\sqrt{1-\xi}} \times \cdots \dots \dots \dots = coskp$$



Brillouin Zone and Number of States

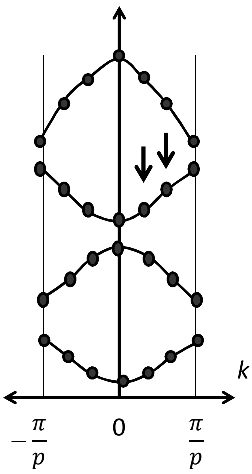


$$k = \pm\frac{2\pi n}{Np} \quad n = -\frac{N}{2}, \ldots -1,0,1, \ldots, \frac{N}{2}$$

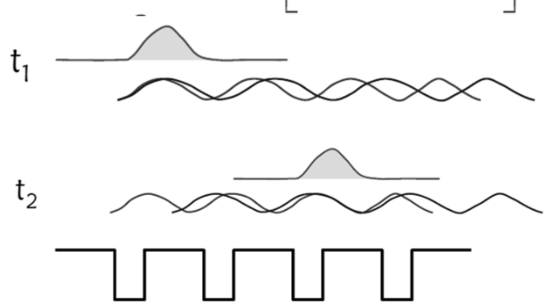
$$\frac{States}{Band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi/p}{2\pi/Np} = N$$

What is the physical meaning of the energy bands?

Wave Packet and Group Velocity



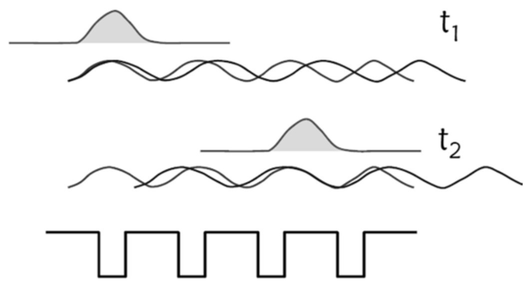
$$\psi(x,t) = Ae^{ikx - i\frac{E}{\hbar}t} + Ae^{i(k+\Delta k)x - i\left(\frac{E+\Delta E}{\hbar}\right)t}$$
$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right]$$



Group Velocity for a Given Band

$$\psi(x,t) = Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right]$$

$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i\times const.}\right]$$



$$\upsilon = \frac{\Delta x}{\Delta t} = \frac{\Delta E}{\hbar \Delta k}$$

$$\because \left[x\Delta k - t\frac{\Delta E}{\hbar}\right] = \text{constant.}$$

$$\boxed{a = \frac{\Delta \upsilon}{\Delta t} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{\Delta E}{\Delta k}\right] = \frac{1}{\hbar^2}\frac{d}{dk}\left[\frac{\Delta E}{\Delta k}\right]\frac{d(\hbar k)}{dt} = \frac{F}{m^*}}$$

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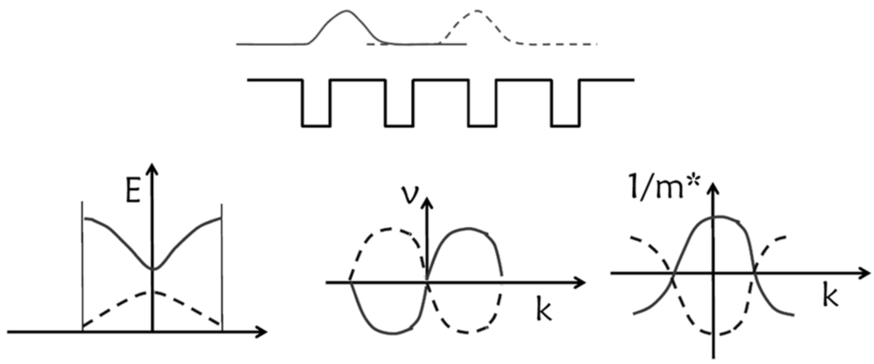
Effective Mass for a Given Band



$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k} \qquad \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2 E}{dk^2}$$

mass for each band

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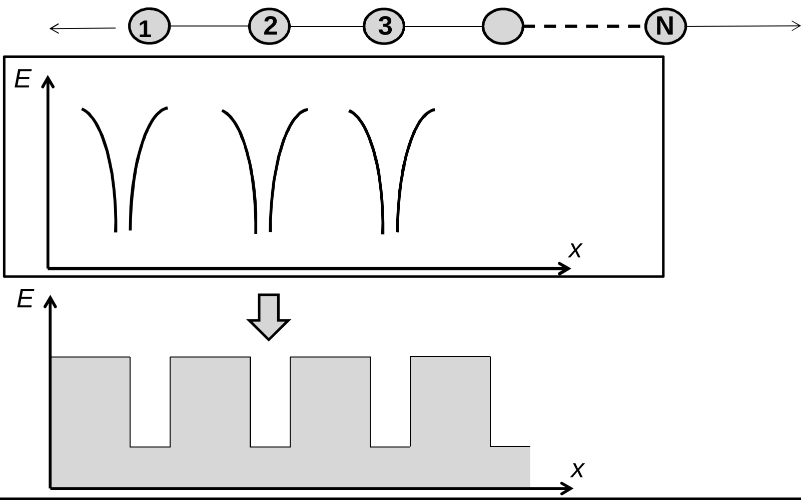
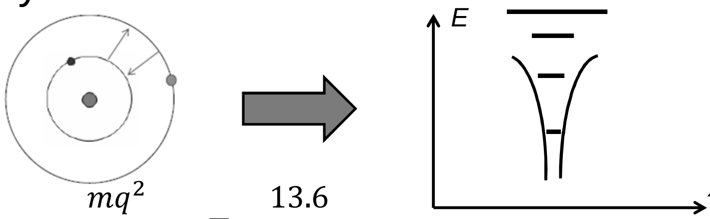
The Physics

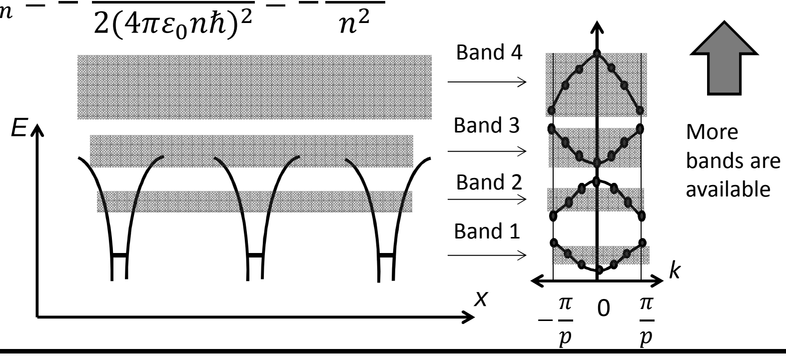


The Physics Cont'd

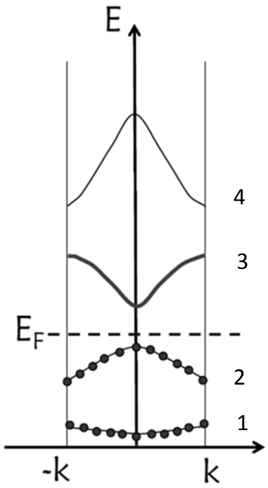
One atom



$$E_n = -\frac{mq^2}{2(4\pi\varepsilon_0 n\hbar)^2} = -\frac{13.6}{n^2}$$



Filled and Empty Bands



No electrons in the empty bands.

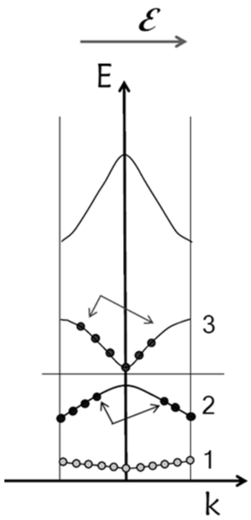
$$J_3 = -\frac{q}{L}\Sigma \sum_{i(filled)}^{N} v_i = 0$$

How about filled bands?

$$J_2 = -\frac{q}{L}\Sigma \sum_{i(filled)}^{N} v_i = -\frac{q}{L}\sum_{0}^{k_{max}} v_i - \frac{q}{L}\sum_{-k_{min}}^{0} v_i = 0$$

Neither filled or empty bands can conduct electricity!

Partially Filled Bands



$$J_3 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i \neq 0$$

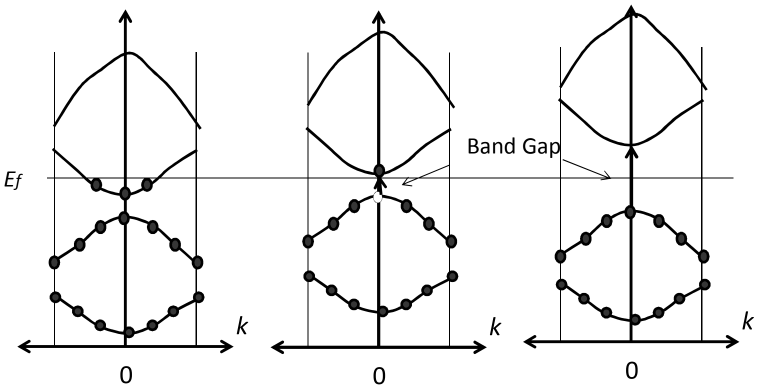
$$J_2 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = \cancel{-\frac{q}{L}\sum_{all} \upsilon_i} + \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

$$= \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

-ve charge moving with –ve mass

+ve charge moving with +ve mass

Metal, Semiconductor, Insulator



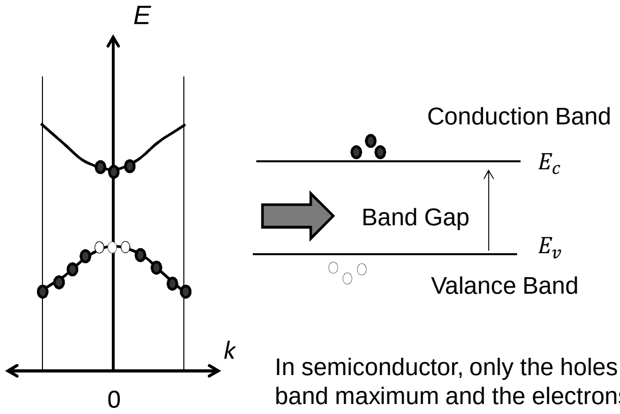
- **Metal:** has partially filled energy bands at zero temperature.
- **Semiconductor:** does not have partially filled bands at zero temperature, but thermal effect can excite electrons into conduction bands.
- **Insulator:** does not have partially filled bands at zero temperature, but band gap energy is too large and thermal effect cannot excite electrons on to conduction bands.

Band Gap Energy

Si ~ 1.12 eV
Ge ~ 0.66 eV
GaAs ~ 1.42 eV

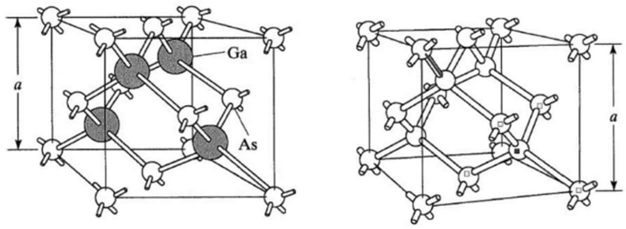
SiO2 ~ 8 eV
Diamond ~ 5 eV

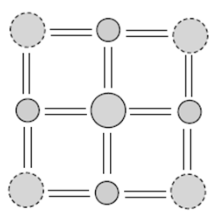
Carriers in the Semiconductor



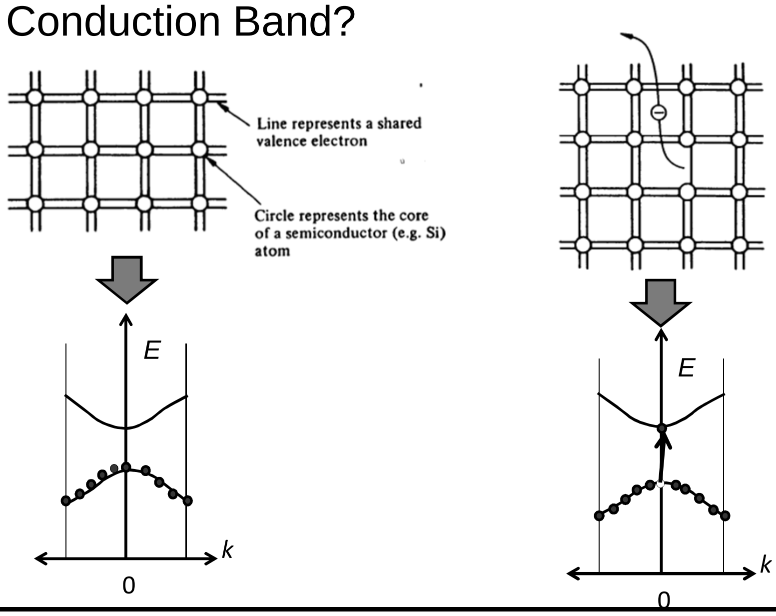
In semiconductor, only the holes near the valance band maximum and the electrons near the conduction band minimum are responsible for conduction.

Simplified Planna View of Atoms

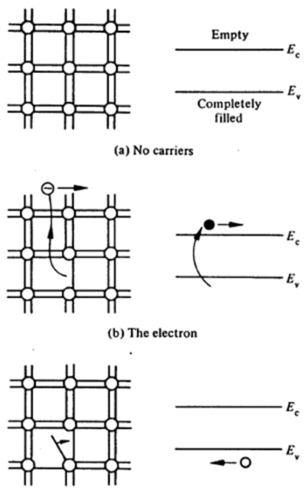




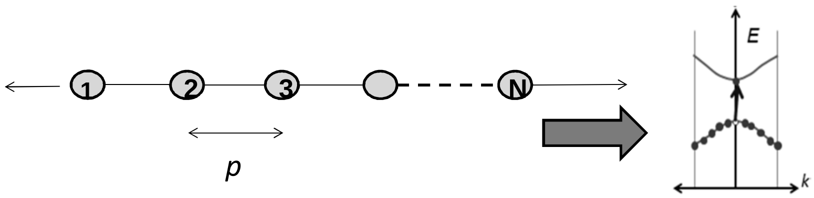
Conduction Band?



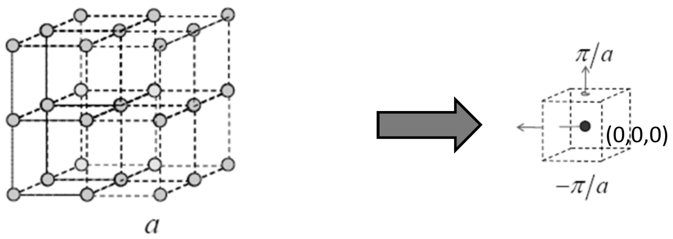
Conduction bands? Holes?



Energy Bands for Real Materials

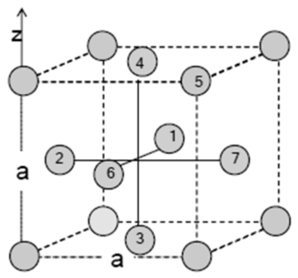


$-\frac{\pi}{p} < k < \frac{\pi}{p}$

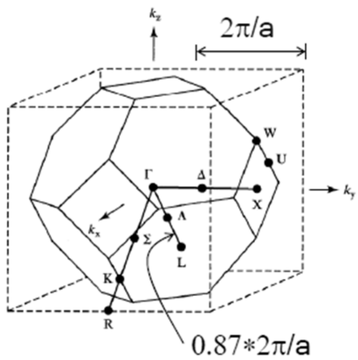


Diamond and zinc-blende structure?

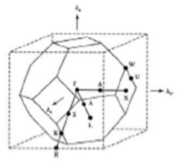
Real Space FCC
(for Si, Ge, GaAs)



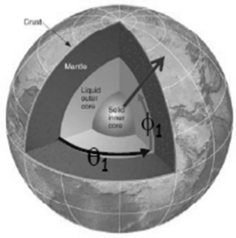
Reciprocal Lattice



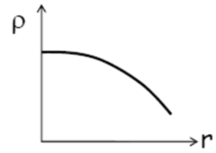
Analog to E-k diagram



Density (x,y,z)
4D information

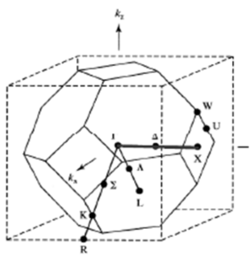


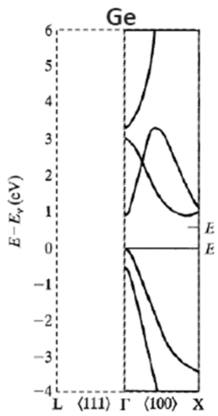
Cut along (θ_1, ϕ_1) ...



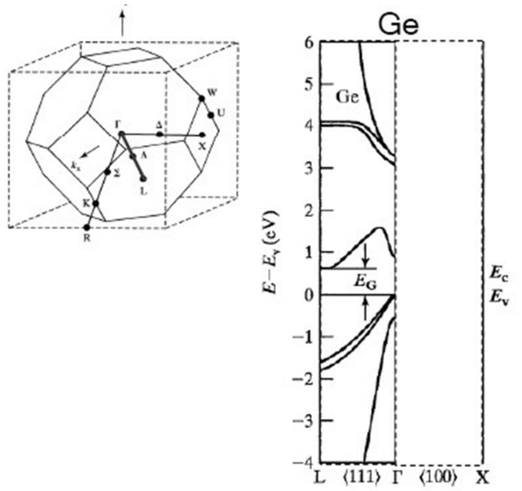
A series of line-sections can
Represent the 4D info in 2D plots

E-k along Γ-X direction

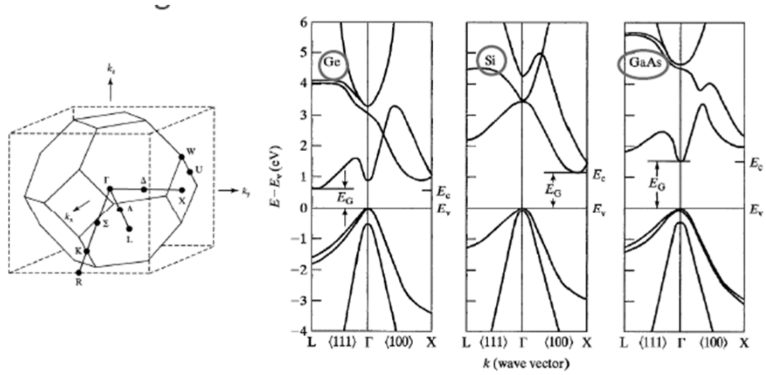




E-k along Γ-L direction



E-k Diagram for Ge, Si, GaAs



- 3 valence bands (light hole, heavy hole, split-off)
  valence bands near k=0 is essentially E ~ k^2
- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: Γ valleys)

Effective Mass

$$a = \frac{\Delta \upsilon}{\Delta t} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{\Delta E}{\Delta k}\right] = \frac{1}{\hbar^2}\frac{d}{dk}\left[\frac{\Delta E}{\Delta k}\right]\frac{d(\hbar k)}{dt} = \frac{F}{m^*}$$

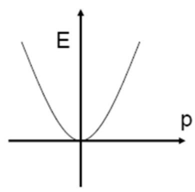
Do not understand?
Let's consider a simpler example…

Free electrons in a vacuum respond to applied electric fields by the following

$$\text{Force} = -q\mathcal{E} = m_0 \frac{dv}{dt} = \frac{dp}{dt}$$

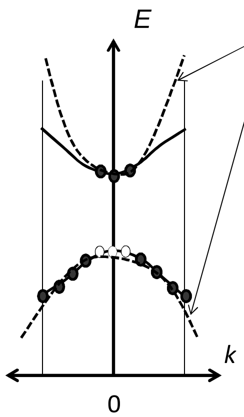
$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

E-p relationship of electron.



$$E = \frac{p^2}{2m_0}$$

Similarly…



The E-k relationship at the conduction band minimum or valance band maximum can be approximated by a parabolic function.

Wave-particle duality:

$$p = \hbar k, \qquad E \approx \frac{p^2}{2m^*}$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

Effective Mass is inversely proportional to the curvature of E-k diagram!

Electrons moving in a solid: $F = -q\mathcal{E} = m_n{}^* \frac{dv}{dt}$

Similar equation for holes: $F = q\mathcal{E} = m_p{}^* \frac{dv}{dt}$

The importance of effective mass

$$F = -q\mathcal{E} = m_n{}^* \frac{dv}{dt}$$

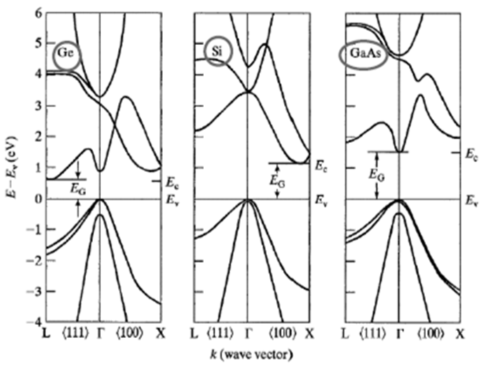
$$F = q\mathcal{E} = m_p{}^* \frac{dv}{dt}$$

Quote from RFP:

"It allows us to conceive of electrons and holes as quasi-classical particles and to employ classical particle relationships in most device analysis! "

Now you can (mostly) forget about quantum mechanics….

Heavy Holes and Light Holes



- There is typically degeneracy at the valence band maximum.
- There could be light holes and heavy holes.

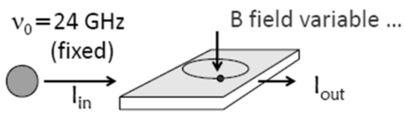
Effective Mass for Semiconductors

Table 2.1 Density of States Effective Masses at 300 K.

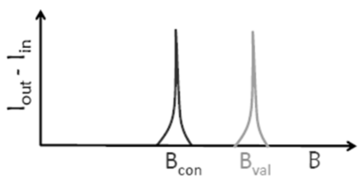
Material	m_n^*/m_0	m_p^*/m_0
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

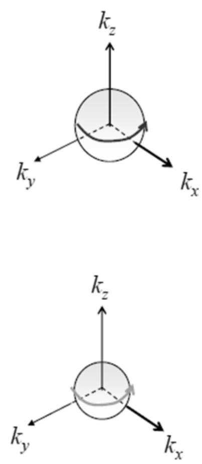
Effective mass is a material property.

Measurement of Effective Mass



$$\nu_0 = \frac{qB_0}{2\pi m^*} \quad m^* = \frac{qB_0}{2\pi \nu_0}$$





Look back …

- We know what the carriers in semiconductors are. (Electrons, holes)
- We know how they moves inside the semiconductor (effective mass)
- But we still do not know how many carriers are there.