ECE606: Solid State Devices
Lecture 4

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Catchup from last lecture

Presentation Outline

- Schrodinger equation in periodic U(x)
- Bloch theorem
- Band structure
- Properties of electronic bands
- E-k diagram and constant energy surfaces
- Conclusions

Reference: Vol. 6, Ch. 3

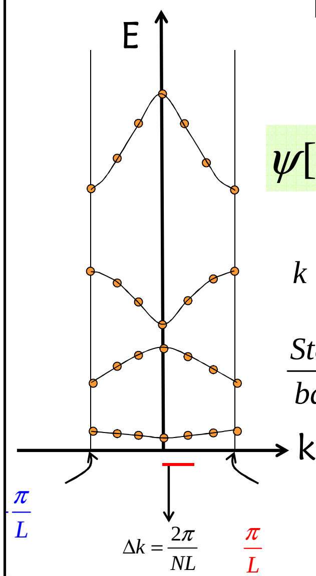
Three Critical Conceptual Steps

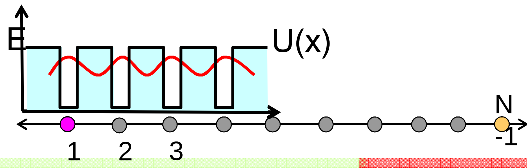
- Basis State Selection
  - » Physical problem is based on a 1D/2D/3D periodic array of atoms
  - » Desired system/signal response is periodic in space
  - » Physical space is infinitely extended
    - ✓ Can the physical space be collapsed into a different representation?
  - » Chose a basis system of plane waves
  - » New finite reciprocal space is representative of the original system
  - » In 2D and 3D the reciprocal space may have critical axes/symmetries
- Solution of the Schroedinger Equation
  - » Solution with plane waves in reciprocal space
  - » 1D solution performed in Kroenig-Penney model (last lecture)
    - ✓ Band formation
  - » 2D/3D solution along critical paths in the reciprocal space
- Filling of the states
  - » States are filled from the bottom up.
  - » Thermal distribution will cause some disorder

Fourier Transform Reminders

$f(x)$	$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-i\omega x}\,dx$	**Space Mapping**
$e^{-a\|x\|}$	$\sqrt{\frac{2}{\pi}}\cdot\frac{a}{a^2+\omega^2}$	**infinite <=> infinite**
$e^{-\alpha x^2}$	$\frac{1}{\sqrt{2\alpha}}\cdot e^{-\frac{\omega^2}{4\alpha}}$	
$\mathrm{rect}(ax)$	$\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}\left(\frac{\omega}{2\pi a}\right)$	**finite <=> infinite**
$\mathrm{tri}(ax)$	$\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}^2\left(\frac{\omega}{2\pi a}\right)$	
1	$\sqrt{2\pi}\cdot\delta(\omega)$	**Periodic => discrete**
e^{iax}	$\sqrt{2\pi}\cdot\delta(\omega-a)$	
$\cos(ax)$	$\sqrt{2\pi}\cdot\frac{\delta(\omega-a)+\delta(\omega+a)}{2}$	

1D Brillouin Zone and Number of States





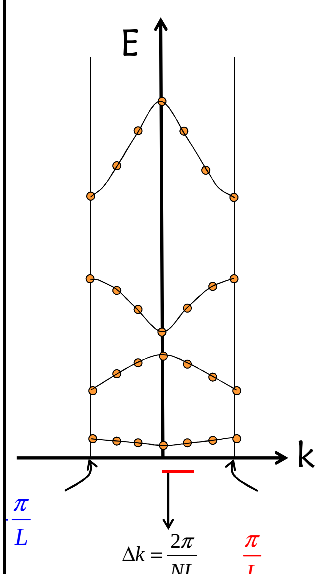
$$\psi[x+NL] = \psi(x)e^{ikLN} = \psi(x)e^{ikLN}e^{i2\pi m}$$
$$= \psi(x)e^{ikLN}e^{imkL}$$

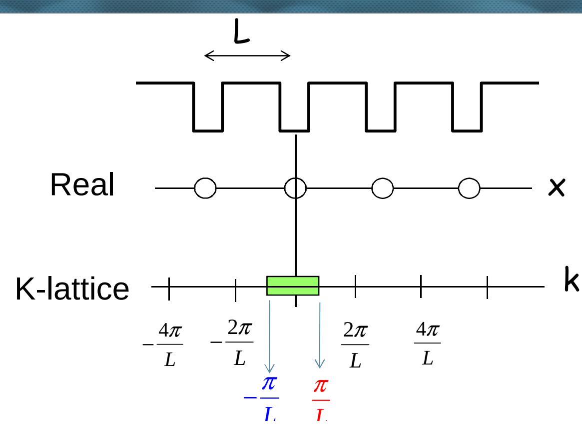
$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2}.....-1,0,1,....\frac{N}{2}$$

$$\frac{States}{band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi/L}{2\pi/NL} = N$$

4 states per atom, N atoms
=> 4 bands, N states in each band
All states are included in the first zone
Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$

Solution Space: Brillouin Zone





4 states per atom, N atoms
=> 4 bands, N states in each band
All states are included in the first zone
Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$
Collapse of an infinite space into a discrete space

Fourier Transform Reminders

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Reciprocal Space

A 1D **periodic** function: $f(x)=f(x+l);\quad l=nL$

can be expanded in a Fourier series:

$$f(x)=\sum_n A_n e^{i2\pi nx/L}=\sum_g A_g e^{igx}\qquad g=\frac{2\pi n}{L}$$

The Fourier components are defined on a discrete set of periodically arranged points (analogy: frequencies) in a reciprocal space to coordinate space.

3D Generalization:

$$u_n(\mathbf{k},\mathrm{r})=\sum_{\mathrm{G}} f_{\mathrm{G}}^{n}(\mathbf{k})e^{i\mathbf{G}\cdot\mathbf{r}};\quad \mathbf{G}=h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3$$

$\mathbf{G}\perp \mathrm{a}$ Where *hkl* are integers. **G**=Reciprocal lattice vector

$$f(\vec{r}) = 1/\sqrt{2\pi} \int d^3\vec{k}\, f(\vec{k}) \exp\left(i\vec{k}\vec{r}\right)$$

Fourier transform:
Represented real-space with plane waves

$$f(\vec{r}+\vec{R}) = f(\vec{r})$$

Impose periodicity in **R**

$$f(\vec{r}+\vec{R}) = 1/\sqrt{2\pi} \int d^3\vec{k}\, f(\vec{k}) \exp\left(i\vec{k}\left(\vec{r}+\vec{R}\right)\right)$$

$$\exp\left(i\vec{k}\vec{R}\right) = 1 \qquad \vec{k}\vec{R} = 2\pi n$$

$$\vec{k} = \vec{G} = h\vec{k}_x + k\vec{k}_x + l\vec{k}_z$$

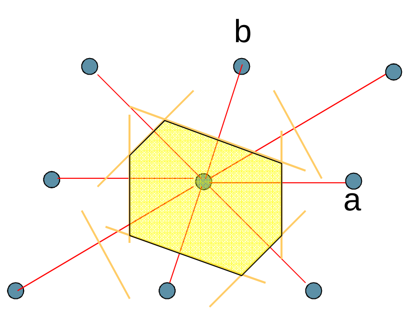
Reciprocal vector **G**

1) Define reciprocal lattice with the following vectors ….

$$k_x = 2\pi \frac{b\times c}{|a\bullet b\times c|} \quad k_y = 2\pi \frac{c\times a}{|a\bullet b\times c|} \quad k_z = 2\pi \frac{a\times b}{|a\bullet b\times c|}$$

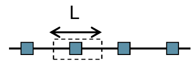
2) Use Wigner Seitz algorithm to find the unit cell in the wave-vector (reciprocal) space.

Primitive cell in real space



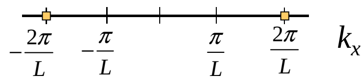
$$k_x = 2\pi \frac{b\times \hat{z}}{|a\bullet b\times \hat{z}|} \quad k_y = 2\pi \frac{\hat{z}\times a}{|a\bullet b\times \hat{z}|}$$

Real-space

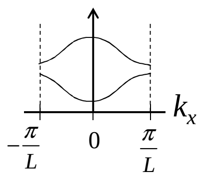


Replacing (a+b) by L …

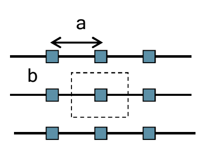
1st B-Z



E-k diagram



Real-space



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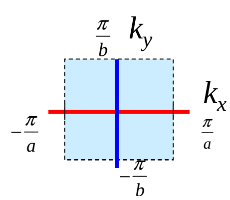
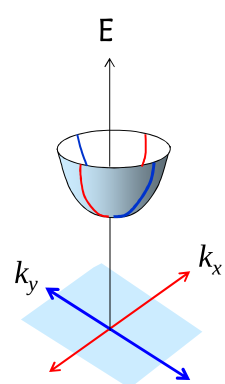


E-k diagram

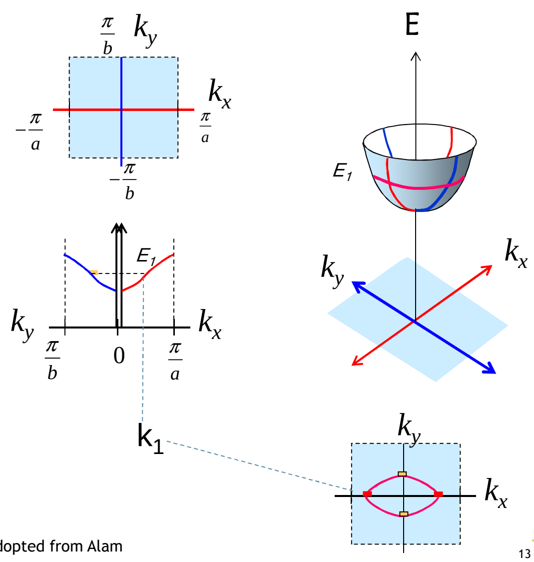


Constant Energy-surface in 2D

1st B-Z

E-k diagram

Const. Energy Surface



Conclusions

- Solution of Schrodinger equation is relatively easy for systems with well-defined periodicity.
- Electrons can only sit in-specific energy bands. Effective masses and band gaps summarize information about possible electronic states.
- Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.
- Kronig-Penney model is analytically solvable. Real band-structures are solved on computer. Such solutions are relatively easy – we will do HW problems on nanohub.org on this topic.
- Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.
- Of all the possible bands, only a few contribute to conduction. These are often called conduction and valence bands.
- For 2D/3D systems, energy-bands are often difficult to visualize. E-k diagrams along specific direction and constant energy surfaces for specific bands summarize such information.
- Most of the practical problems can only be analyzed by numerical solution.

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- Reminder – bandstructure in 1D – Brillouin Zone
- E-k diagram/constant energy surfaces in 3D solids
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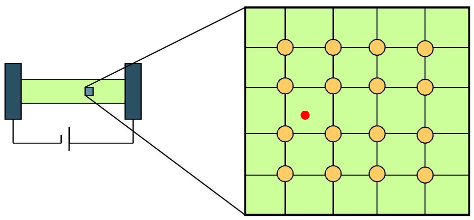
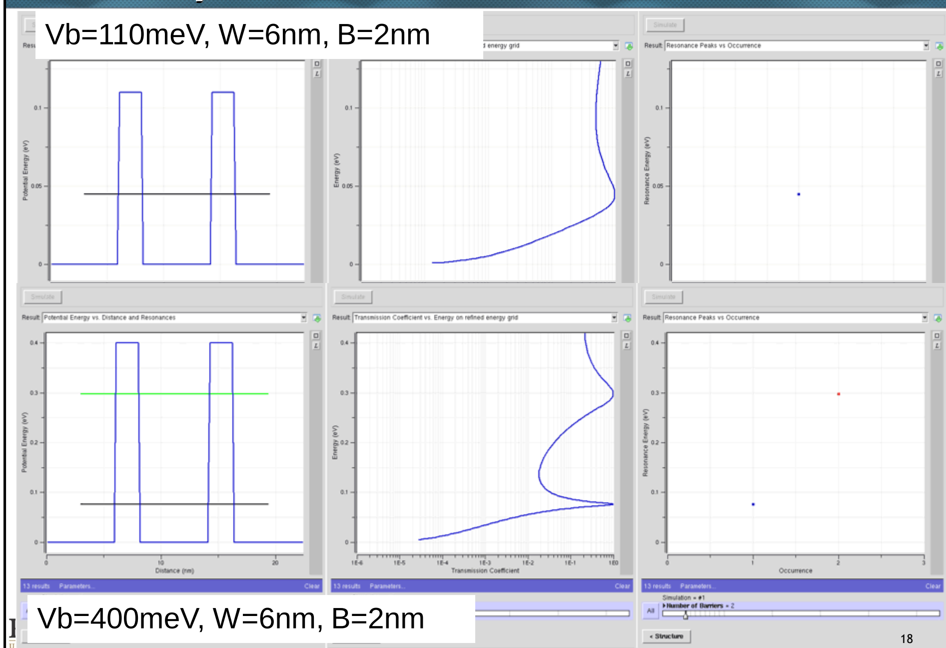
How do electrons move through a real crystal?



N Wells => 2N States => 2 Bands

Vb=110meV, W=6nm, B=2nm



Vb=400meV, W=6nm, B=2nm

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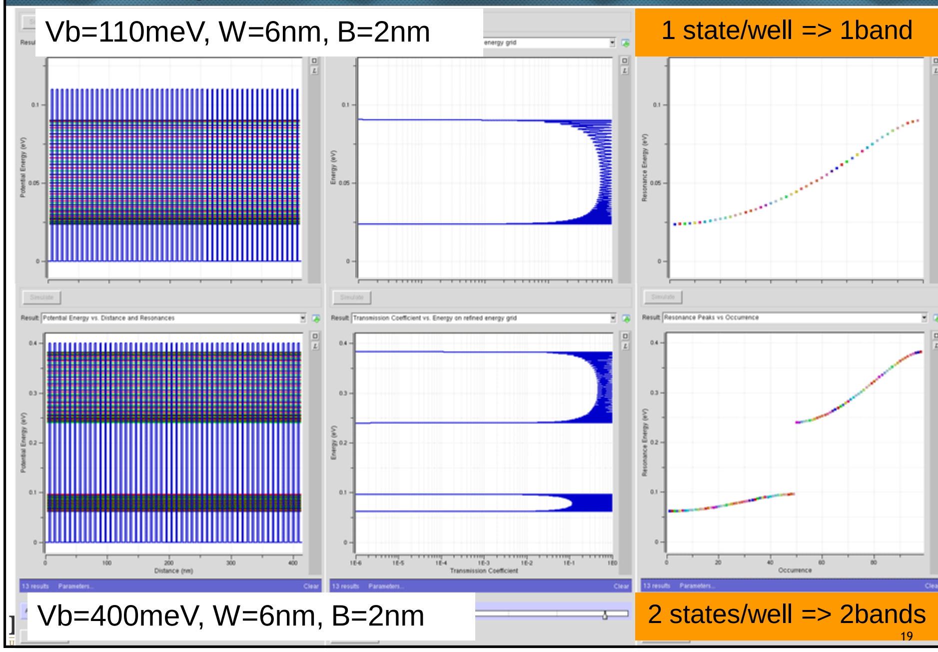
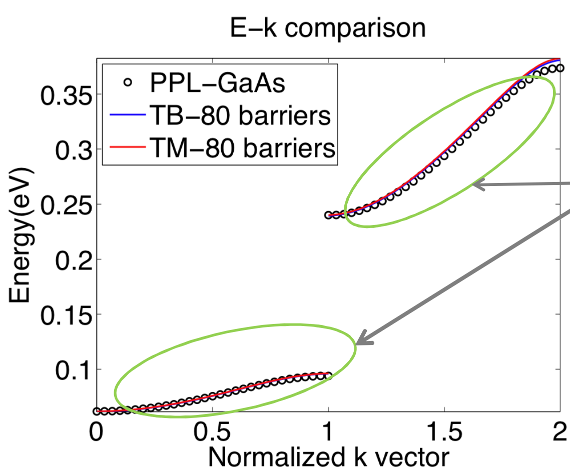


GaAs Well Comparison - 80 Barriers

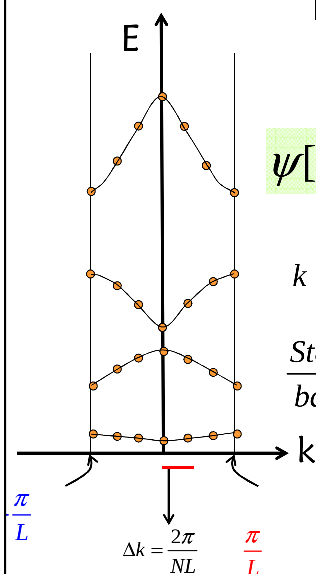


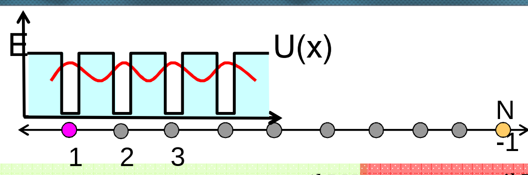
A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 80 barriers using tight-binding.
- TM: 80 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.

Brillouin Zone and Number of States





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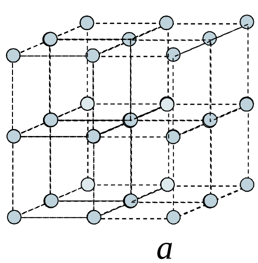
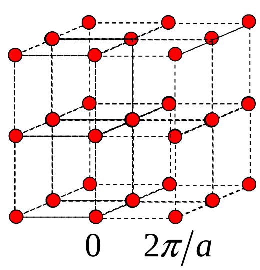
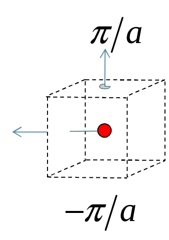
Real Space Cubic Lattice



Reciprocal Lattice

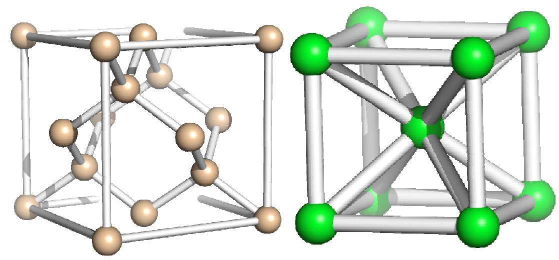


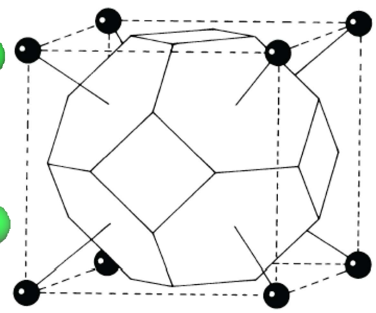
Brillouin Zone



Follow W-S algorithm, but now for reciprocal lattice

Real Space FCC (for Si, Ge, GaAs) **Reciprocal Lattice** **Brillouin Zone of Reciprocal Lattice**





Diamond lattice and bcc are Fourier Transforms of each other!

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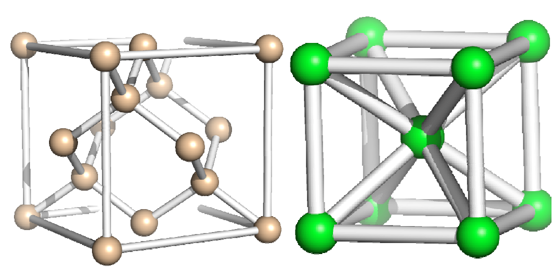
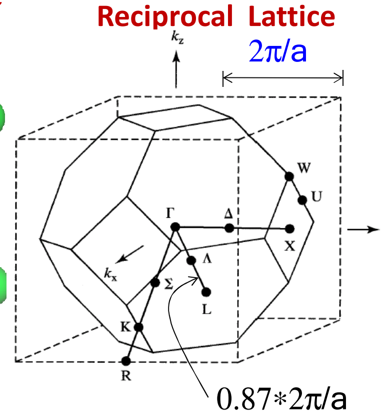
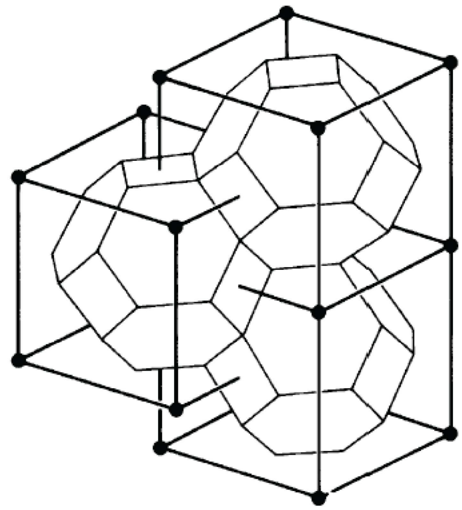




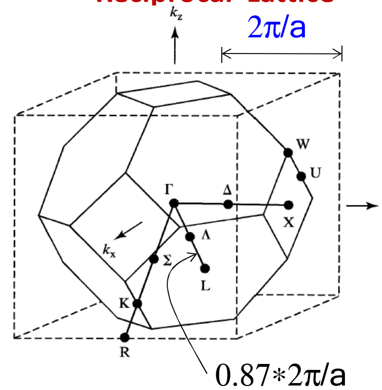
Diamond lattice and bcc are Fourier Transforms of each other!

Note unlike cubic lattice, zone edge is not at π/a

Brillouine Zone is Space Filling



Brillouin Zone of Reciprocal Lattice



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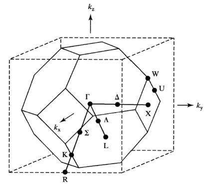
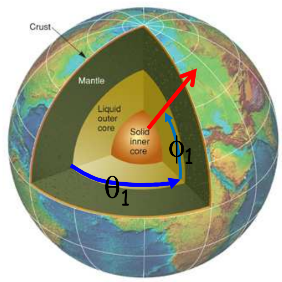
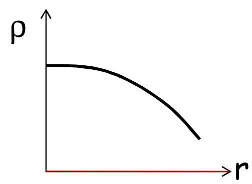
Analogy for E-k Diagram: 4D info thiough 2D Plots



Density (x,y,z)
4D information

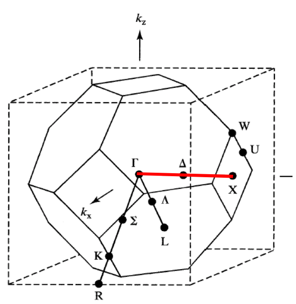


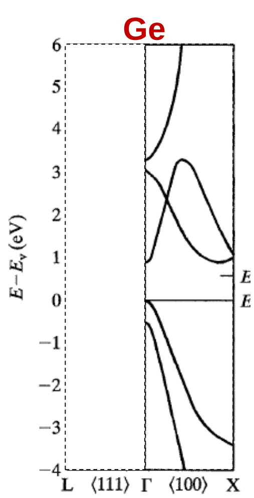
Cut along (θ_1, ϕ_1) …



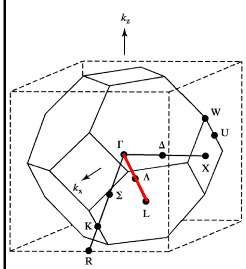
A series of line-sections can
Represent the 4D info in 2D plots

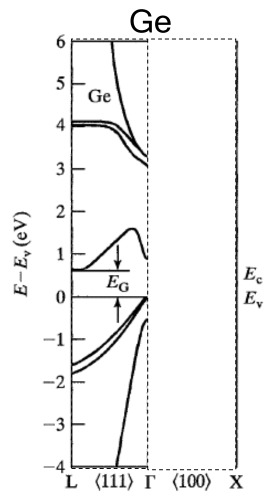
E-k along Γ-X Direction



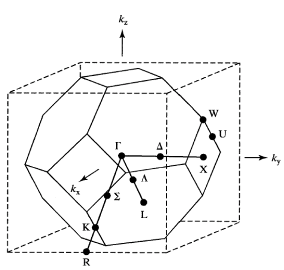


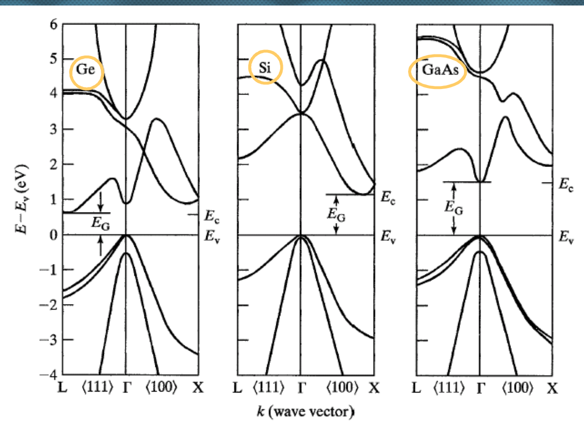
E-k along Γ-L direction





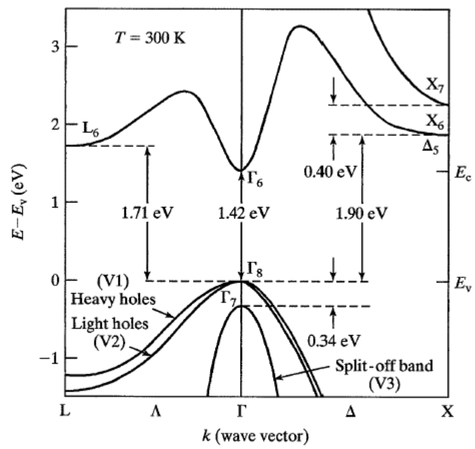
E-k Diagram





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

E-k diagram for GaAs

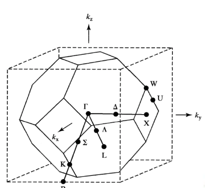


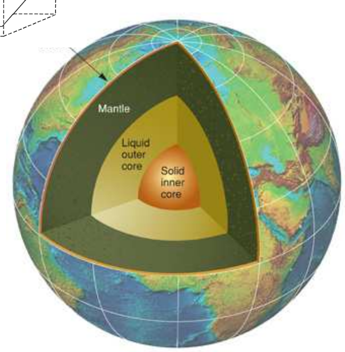
Direct bandgap material

Zone-edge gaps (L_6-Γ_8, X_6-Γ_8) close to direct gap

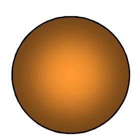
Has important implications
For transport

Analogy for E-k Diagram





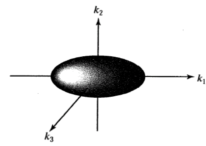
Contours of density ….



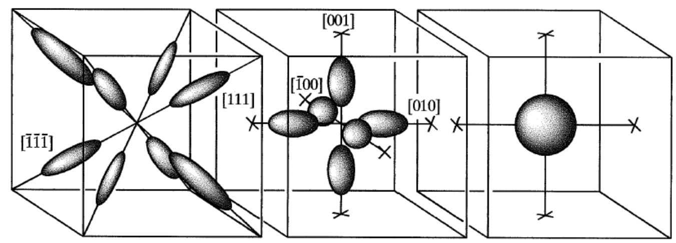
Density (x,y,z)

Constant-E surface for Conduction Band

$E = E_c + Ak_1^2 + B(k_2^2 + k_3^2)$



$E = E_c + A(k_1^2 + k_2^2 + k_3^2)$



Ge (a) Si (b) GaAs (c)

Constant E-surface …

$E = E_c + {\color{red}A}k_1^2 + {\color{blue}B}(k_2^2 + k_3^2)$

$E = E_c + {\color{red}A}(k_1^2 + k_2^2 + k_3^2)$

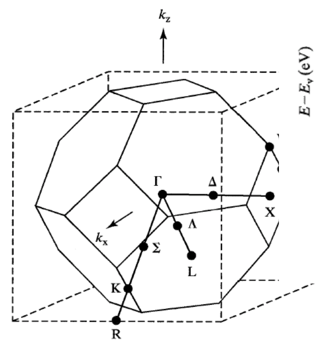
$$\frac{1}{m_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

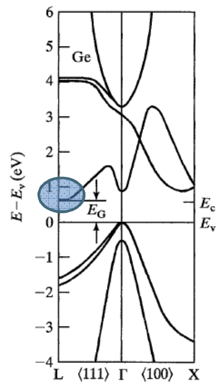
$$\frac{1}{m_{11}} = \frac{{\color{red}2A}}{\hbar^2};\ \frac{1}{m_{22}} = \frac{1}{m_{33}} = \frac{{\color{blue}2B}}{\hbar^2};\ \frac{1}{m_{ij}(i \neq j)} = 0$$

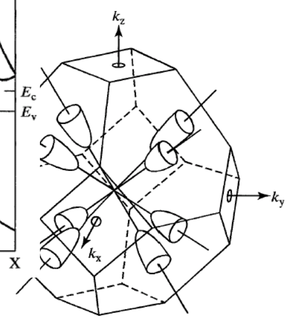
$$\frac{1}{m_{11}} = \frac{1}{m_{22}} = \frac{1}{m_{33}} = {\color{red}2A};\ \frac{1}{m_{ij}(i \neq j)} = 0$$

Offdiagonal Elements=0
=> Force and movement aligned

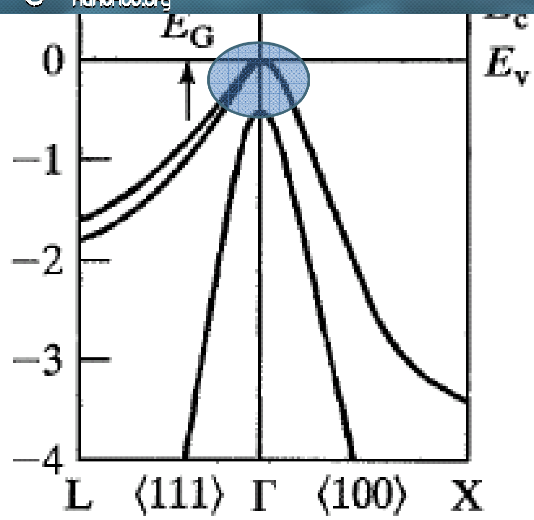
Four valleys inside BZ for Germanium

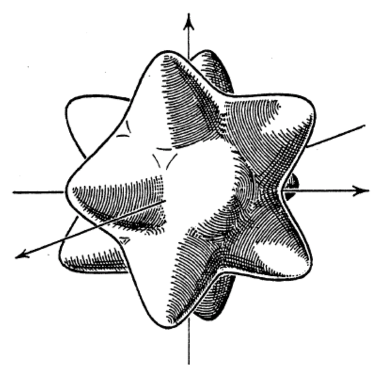






Constant E-surface for Valence Band





$$E = E_v - Ak^2 \mp \sqrt{[B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)]}$$

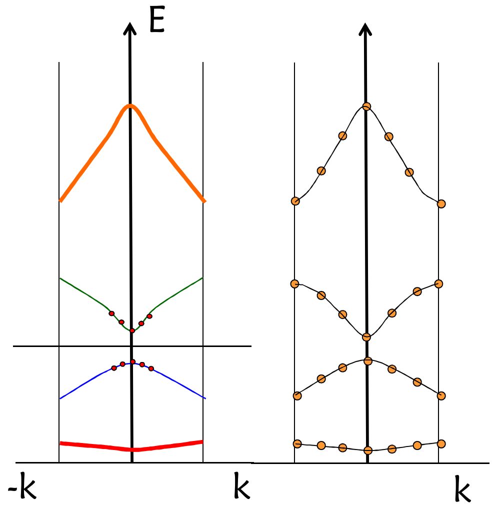
Si: A=4.29, B=0.68, C=4.87; Ge: A=13.38, B=8.48, C=13.15

Presentation Outline

- Reminder – bandstructure in 1D – Brillouin Zone
- E-k diagram/constant energy surfaces in 3D solids
- **Definition of a density of states**
- Density of States for specific materials
- Conclusions

Reference: Vol. 6, Ch. 3

Density of States



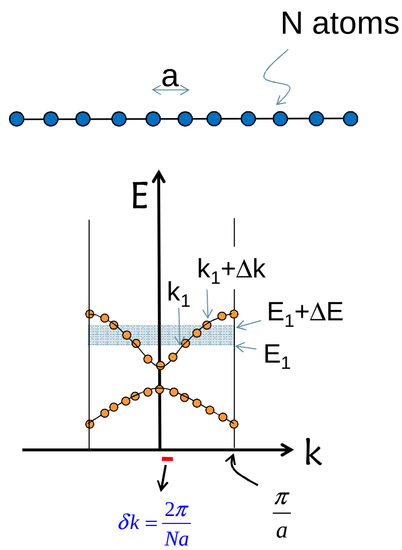
A single band has total of N-states

Only a fraction of states are occupied

How many states are occupied up to E?

Or equivalently…

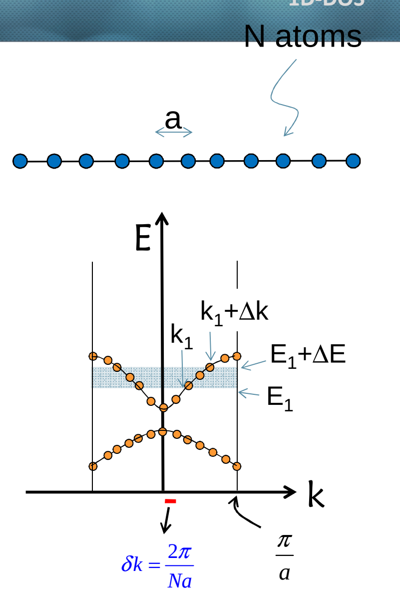
How many states per unit energy ? (DOS)



$$\text{States between } E_1+\Delta E \;\&\; E_1 = 2\times\frac{\Delta k}{\delta k}$$

$$= 2\times\frac{\Delta k}{2\pi/Na}$$

$$\text{States/unit energy @ } E_1 = \frac{Na}{\pi}\frac{\Delta k}{\Delta E}$$



L

$$\text{States/unit energy @ } E = \frac{Na}{\pi}\frac{\Delta k}{\Delta E}$$

$$E - E_0 = \frac{\hbar^2 k^2}{2m^*} \Rightarrow k = \sqrt{\frac{2m^*(E-E_0)}{\hbar^2}}$$

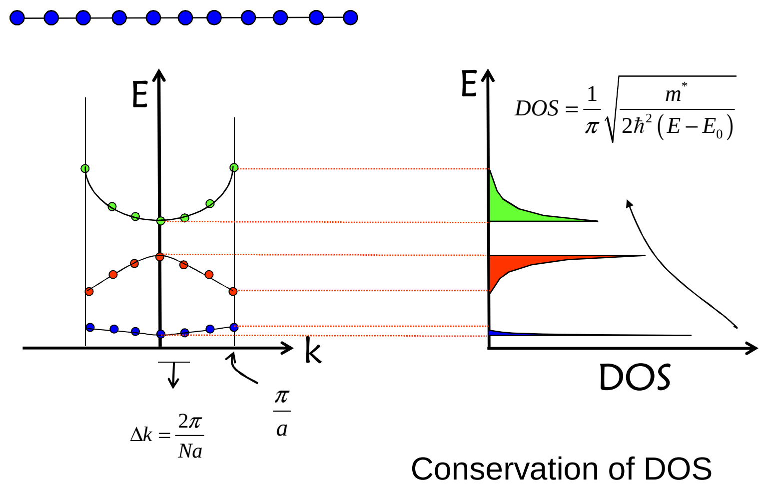
$$\frac{dk}{dE} = \sqrt{\frac{m^*}{2\hbar^2(E-E_0)}}$$

$$\text{States/unit energy @ } E = \frac{L}{\pi}\sqrt{\frac{m^*}{2\hbar^2(E-E_0)}}$$

States/unit energy/unit length @ E

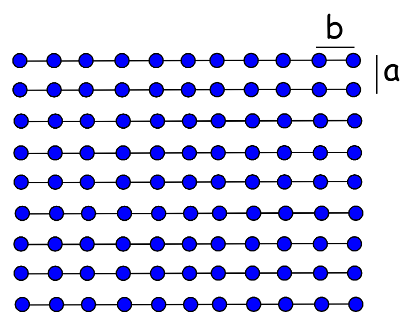
$$\equiv DOS = \frac{1}{\pi}\sqrt{\frac{m^*}{2\hbar^2(E-E_0)}}$$

1D-DOS



Conservation of DOS

Density of States in 2D Semiconductors

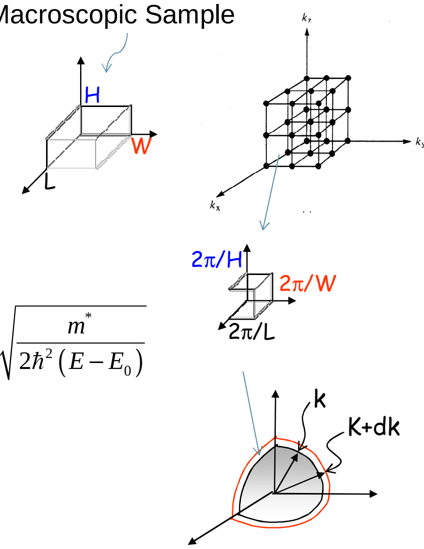


Show that 2D DOS is a constant independent of energy!

States between $E_1+\Delta E$ & E_1

$$=\frac{\frac{4}{3}\pi(k+dk)^3-\frac{4}{3}\pi k^3}{\frac{2\pi}{L}\frac{2\pi}{W}\frac{2\pi}{H}}=\frac{V}{2\pi^2}k^2\Delta k$$

Macroscopic Sample



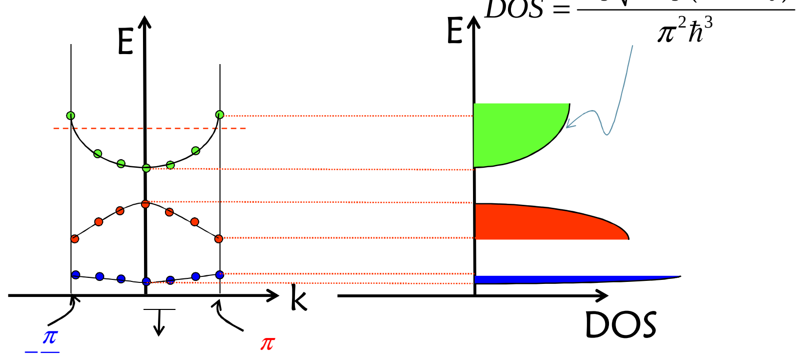
States/unit energy @ E $=\frac{V}{2\pi^2}k^2\frac{\Delta k}{dE}$

$$E-E_0=\frac{\hbar^2k^2}{2m^*}\Rightarrow k=\sqrt{\frac{2m^*(E-E_0)}{\hbar^2}}\Rightarrow\frac{dk}{dE}=\sqrt{\frac{m^*}{2\hbar^2(E-E_0)}}$$

States/unit energy/unit volume @ E_1

$$DOS=\frac{m^*}{2\pi^2\hbar^3}\sqrt{2m^*(E-E_0)}$$

$$DOS=\frac{m_3^*\sqrt{2m_3^*(E-E_0)}}{\pi^2\hbar^3}$$



$-\frac{\pi}{a}$ $\quad \Delta k=\frac{2\pi}{Na}$ $\quad \frac{\pi}{a}$

Conservation of DOS

Presentation Outline

- Reminder – bandstructure in 1D – Brillouin Zone
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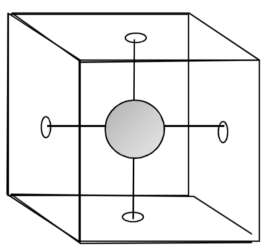
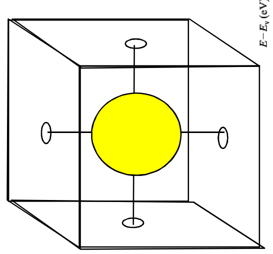
Reference: Vol. 6, Ch. 3

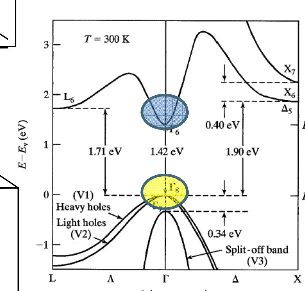
Density of States of GaAs: Conduction/Valence Bands

$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E-E_c)}}{2\pi^2\hbar^3}$$

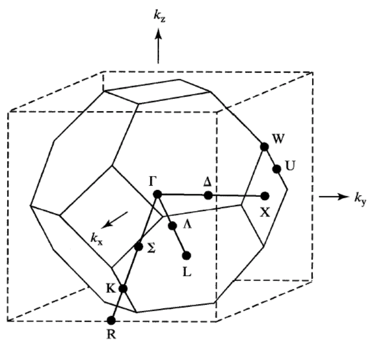


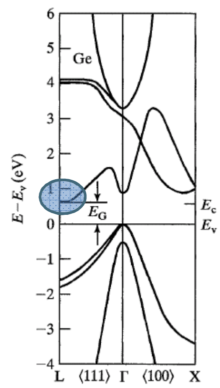
$$g_\upsilon(E) = \begin{cases} \dfrac{m_{hh}^* \sqrt{2m_{hh}^*(E-E_\upsilon)}}{2\pi^2\hbar^3} \\ \dfrac{m_{lh}^* \sqrt{2m_{lh}^*(E-E_\upsilon)}}{2\pi^2\hbar^3} \end{cases}$$

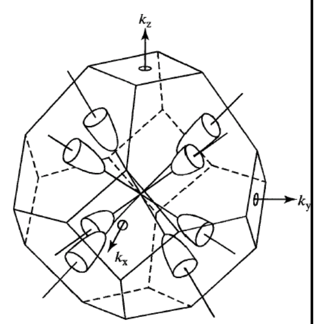




Four valleys inside BZ for Germanium



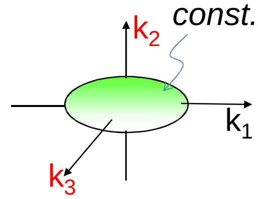




Ellipsoidal Bands and DOS Effective Mass

$$E - E_C = \frac{\hbar^2 k_1^2}{2m_l^*} + \frac{\hbar^2 k_2^2}{2m_t^*} + \frac{\hbar^2 k_3^2}{2m_t^*}$$

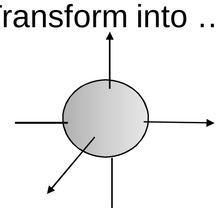
E=const. ellipsoid



$$1 = \frac{k_1^2}{\left[\frac{2m_l^*(E-E_C)}{\hbar^2}\right]} + \frac{k_2^2}{\left[\frac{2m_t^*(E-E_C)}{\hbar^2}\right]} + \frac{k_3^2}{\left[\frac{2m_t^*(E-E_C)}{\hbar^2}\right]}$$

α^2 β^2

Transform into …



$$\mathcal{V}_k = N_{el}\left(\frac{4}{3}\pi\alpha\beta^2\right) \equiv \frac{4}{3}\pi k_{eff}^3$$

$$N_{el}\frac{4}{3}\pi\sqrt{\frac{2m_l^*(E-E_c)}{\hbar^2}}\sqrt{\frac{2m_t^*(E-E_c)}{\hbar^2}}\sqrt{\frac{2m_t^*(E-E_c)}{\hbar^2}} \equiv \frac{4}{3}\pi\left[\sqrt{\frac{2m_{eff}^*(E-E_c)}{\hbar^2}}\right]^3$$

$$m_{eff}^* = N_{el}^{2/3}\left(m_l^* m_t^{*2}\right)^{1/3}$$

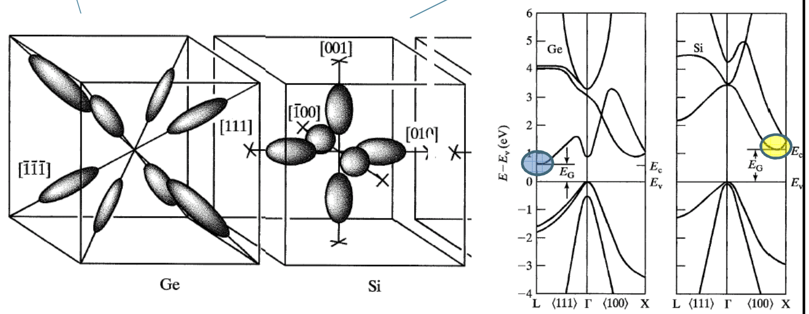
N_{el} is number of equivalent ellipsoids

$$m_{eff}^{*} = 4^{2/3}\left(m_l^{*} m_t^{*2}\right)^{1/3}$$

$$g_c(E) = \frac{m_{eff}^{*}\sqrt{2m_{eff}^{*}(E-E_c)}}{2\pi^2\hbar^3}$$

$$m_{eff}^{*} = 6^{2/3}\left(m_l^{*} m_t^{*2}\right)^{1/3}$$

$$g_c(E) = \frac{m_{eff}^{*}\sqrt{2m_{eff}^{*}(E-E_c)}}{2\pi^2\hbar^3}$$



1) E-k diagram/constant energy surfaces are simple ways to represent the locations where electrons can sit. They arise from the solution of Schrodinger equation in periodic lattice.
2) E-k diagram and energy bands contain equivalent information. In principle, any one can be used to construct the other.
3) Only a fraction of the available states are occupied. The number of available states change with energy. DOS captures this variation.
4) DOS is an important and useful characteristic of a material that should be understood carefully.

ECE606: Solid State Devices
Lecture 6

Gerhard Klimeck
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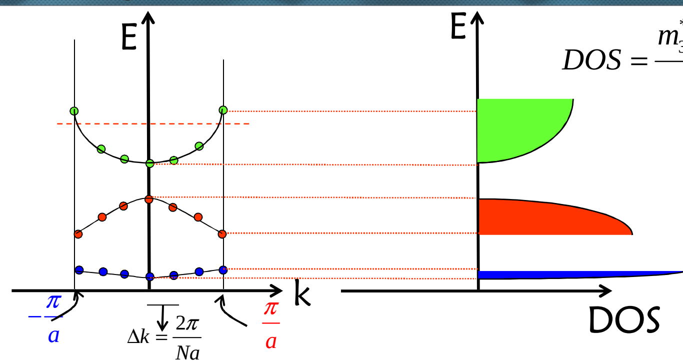
- Reminder – Density of states
  - »Possible states as a function of Energy
- Reality check - Measurements of Bandgaps
- Reality check - Measurements of Effective Mass
- Rules of filling electronic states
- Derivation of Fermi-Dirac Statistics: three techniques
- Intrinsic carrier concentration
- Conclusions

Reference: Vol. 6, Ch. 3 & 4

Reminder: Momentum vs. DOS

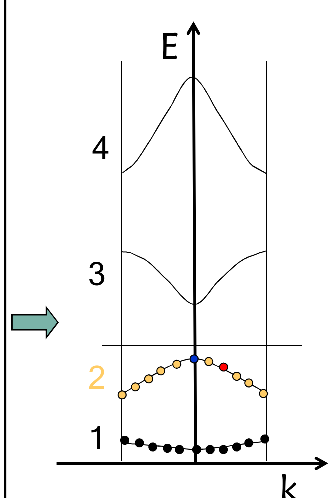


$$DOS = \frac{m_3^* \sqrt{2m_3^*\left(E - E_0\right)}}{\pi^2 \hbar^3}$$

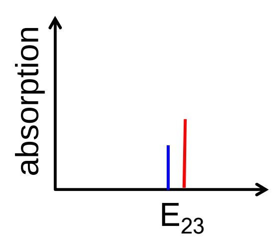
Important things to remember:

- Momentum k entered our thinking as a quantum number
- Each quantum number is creating ONE state
- Often “just” need the number of available states in an energy range
  => Density of States
  => appears to be solely determined by
  - 1) band edge,
  - 2) effective mass

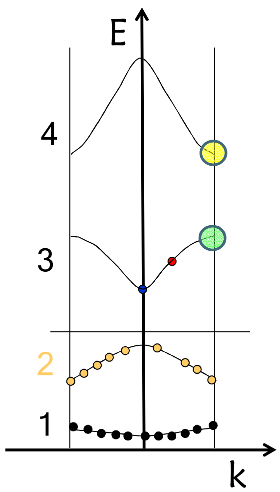
Measurement of Band Gap

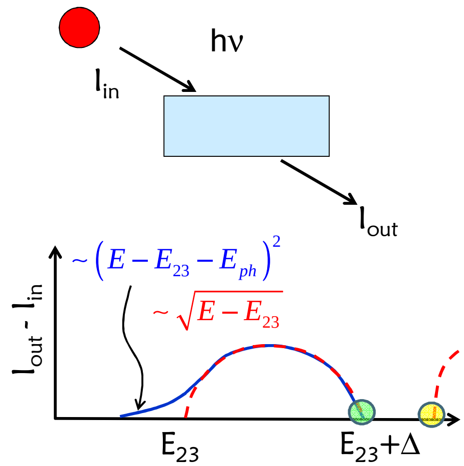


Photons are only absorbed between bands that have filled and empty states



Measurement of Energy Gap





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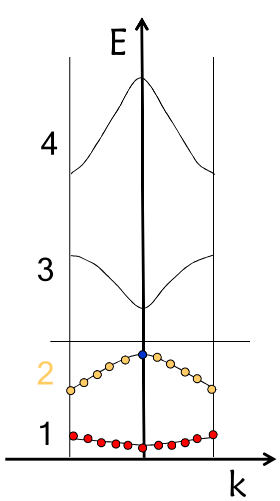
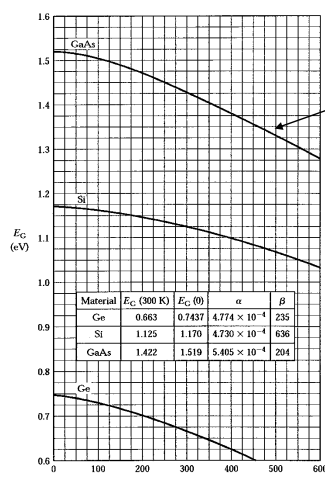
Temperature-dependent Band Gap





Material	E_C (300 K)	E_C (0)	α	β
Ge	0.663	0.7437	4.774×10^{-4}	235
Si	1.125	1.170	4.730×10^{-4}	636
GaAs	1.422	1.519	5.405×10^{-4}	204

$$E_G(T) = E_G(0) - \frac{\alpha T^2}{T + \beta}$$

Klimeck - ECE606 Fall 2012 - notes adopted from Alam

Presentation Outline

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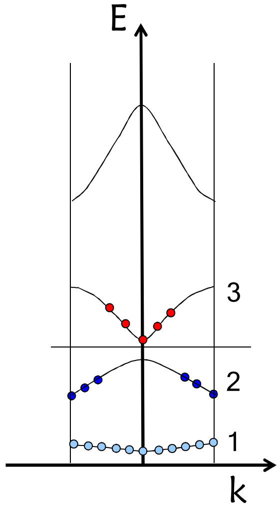
Measurements of Effective Masses



Important things to remember:

- Full bands do not conduct – electrons have no space to go
- Empty bands to not conduct – there are no electrons to go around

Question:

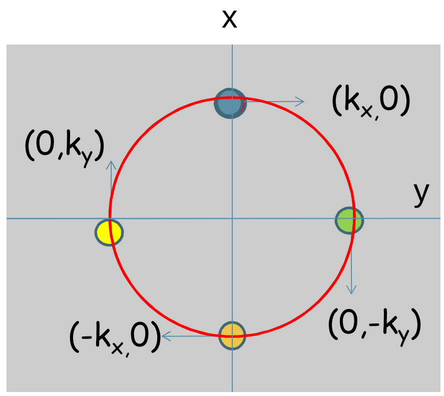
- We are interested in the top-most valence band holes and the bottom-most electron states
- We want to figure out the slope of the bands
- How can we probe just one particular species of electrons/holes?
- We do not want to transfer them from one band to the next!

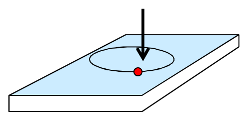
=> can we rotate the electrons around in a single band?

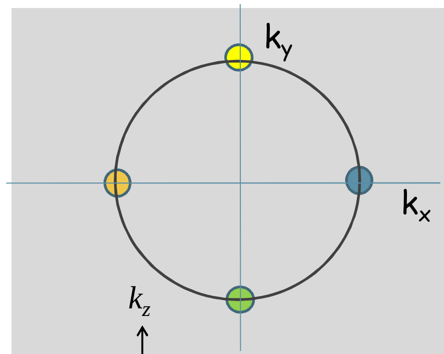
Motion in Real Space and Phase Space

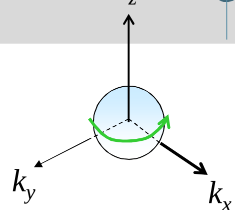
Energy=constant.

Liquid He temperature …









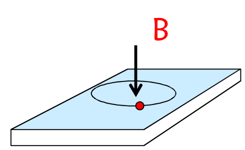
Derive the Cyclotron Formula

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

For an particle in (x-y) plane with B-field in z-direction, the Lorentz force is …

$$\frac{m^* \upsilon^2}{r_0} = q\upsilon \times B_z = q\upsilon B_z$$

$$\upsilon = \frac{qB_0 r_0}{m^*}$$

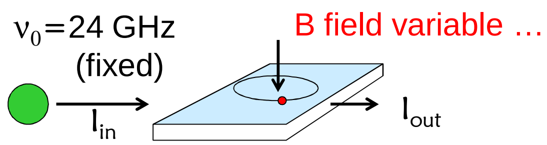


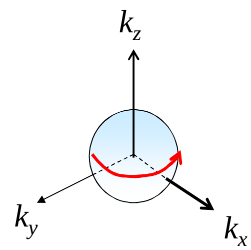
$$\tau = \frac{2\pi r_0}{\upsilon} = \frac{2\pi m^*}{qB_0}$$

$$\nu_0 \equiv \frac{1}{\tau} = \frac{qB_0}{2\pi m^*}$$

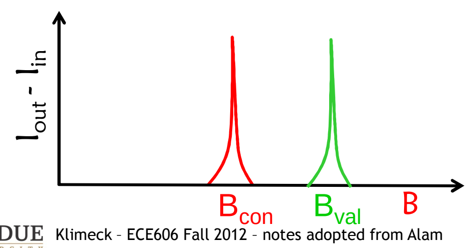
$$\omega_0 = 2\pi\nu_0 = \frac{qB_0}{m^*}$$

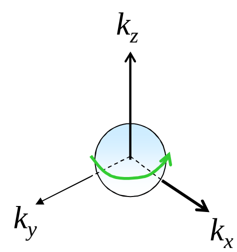
Measurement of Effective Mass



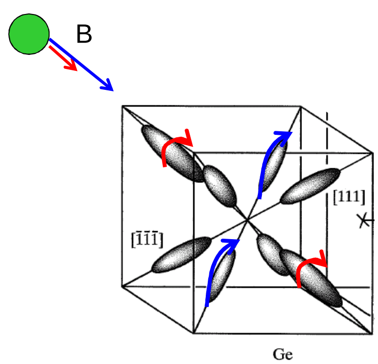


$$\nu_0 = \frac{qB_0}{2\pi m^*} \qquad m^* = \frac{qB_0}{2\pi \nu_0}$$





Effective mass in Ge



$[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}1\bar{1}]$ $[1\bar{1}\bar{1}]$

$[1\bar{1}\bar{1}]$ $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[111]$

4 angles between B field and the ellipsoids …
Recall the HW1

Derivation for the Cyclotron Formula

Show that $$\frac{1}{m_c^{\,2}} = \frac{cos^2\theta}{m_t^{\,2}} + \frac{sin^2\theta}{m_l m_t}$$

Given three m_c and three θ, we will Find m_t, and m_l

The Lorentz force on electrons in a B-field

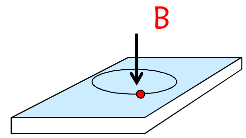
$$F = q\upsilon \times B = [M]\frac{d\upsilon}{dt}$$

In other words,

$$F_x = q\left(\upsilon_y B_z - \upsilon_z B_y\right) = m_t^*\frac{d\upsilon_x}{dt}$$

$$F_y = q\left(\upsilon_z B_x - \upsilon_x B_z\right) = m_t^*\frac{d\upsilon_y}{dt}$$

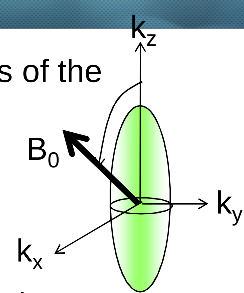
$$F_z = q\left(\upsilon_x B_y - \upsilon_y B_x\right) = m_l^*\frac{d\upsilon_z}{dt}$$



Continued …

Let (B) make an angle (θ) with longitudinal axis of the ellipsoid (ellipsoids oriented along k_z)

$$B_x = B_0\, cos(\theta),\; B_y = 0,\; B_z = B_0\, sin(\theta),$$

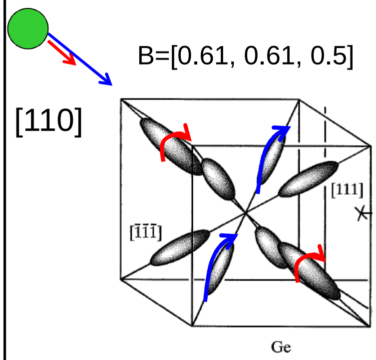


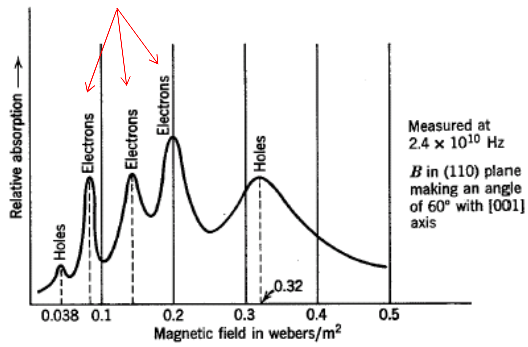
Differentiate (v_y) and use other equations to find …

$$\frac{d^2\upsilon_y}{dt^2} + \upsilon_y\omega^2 = 0 \quad \text{with} \quad \omega^2 \equiv \left[\omega_t w_l\, sin^2\theta + \omega_t^2 cos^2\theta\right]$$

$$\omega_0 \equiv \frac{qB_0}{m_c^*} \qquad \omega_t \equiv \frac{qB_0}{m_t^*} \qquad \omega_l \equiv \frac{qB_0}{m_l^*}$$

so that … $$\frac{1}{\left(m_c^*\right)^2} = \frac{sin^2\theta}{m_l m_t} + \frac{cos^2\theta}{m_t^{\,2}}$$



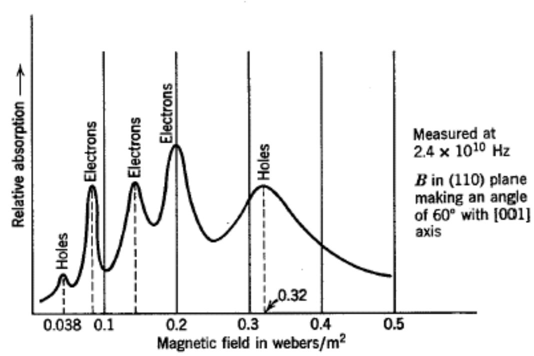


$$\frac{1}{m_c^2} = \frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_l m_t}$$

Three peaks B_1, B_2, B_3
Three masses m_{c1}, m_{c2}, m_{c3}
Three unique angles: 7, 65, 73

$$m_c = \frac{qB_1}{2\pi\nu_0}$$

Known θ and m_c allows calculation of m_t and m_l.



Which peaks relate to valence band?
Why are there two valence band peaks?

Conclusions

1) Only a fraction of the available states are occupied. The number of available states change with energy. DOS captures this variation.
2) DOS is an important and useful characteristic of a material that should be understood carefully.
3) Experimental measurements are key to making sure that the theoretical calculations are correct. We will discuss them in the next class.