PURDUE UNIVERSITY

NCN

www.nanohub.org

EE-606: Solid State Devices

Lecture 7: Energy Bands in Real Crystals

Muhammad Ashraful Alam
alam@purdue.edu

Outline

1) **E-k diagram/constant energy surfaces in 3D solids**

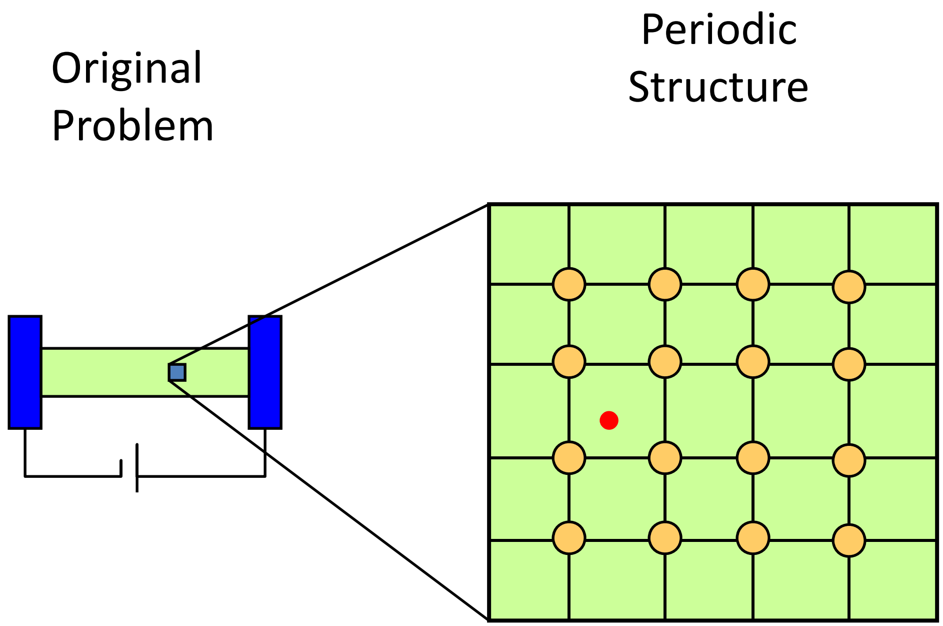
2) Characterization of E-k diagram: Bandgap

3) Characterization of E-k diagram: Effective Mass

4) Conclusions

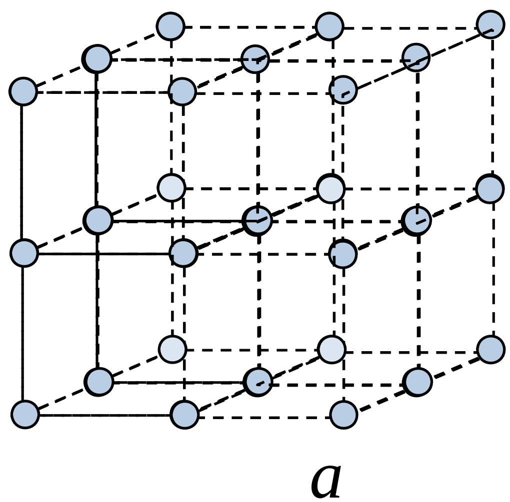
Reference: Vol. 6, Ch. 3 (pages 71-77)

Electronic States

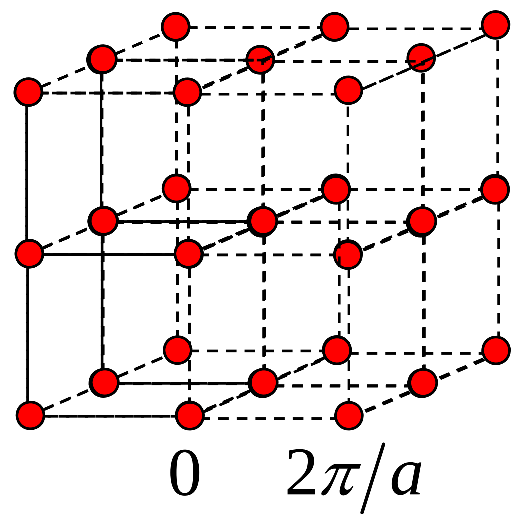


Brillouin Zone in Cubic Lattice …

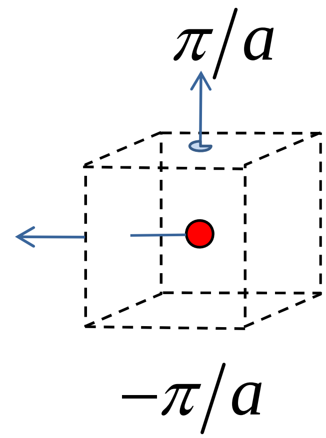
Real Space Cubic Lattice



Reciprocal Lattice



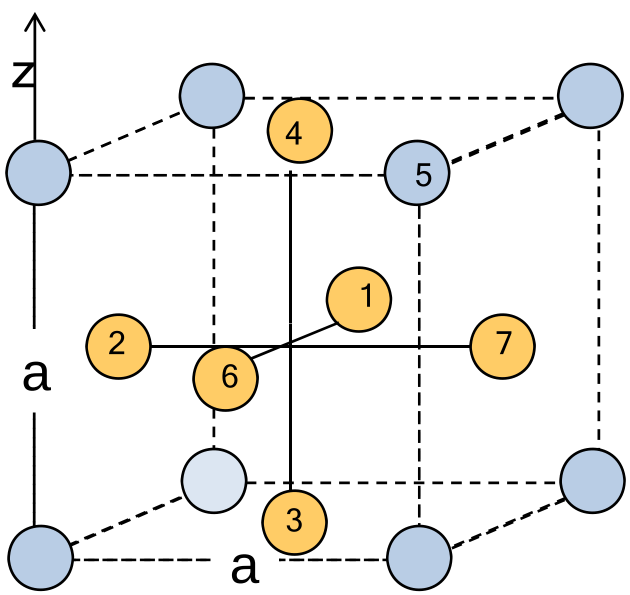
Brillouin Zone



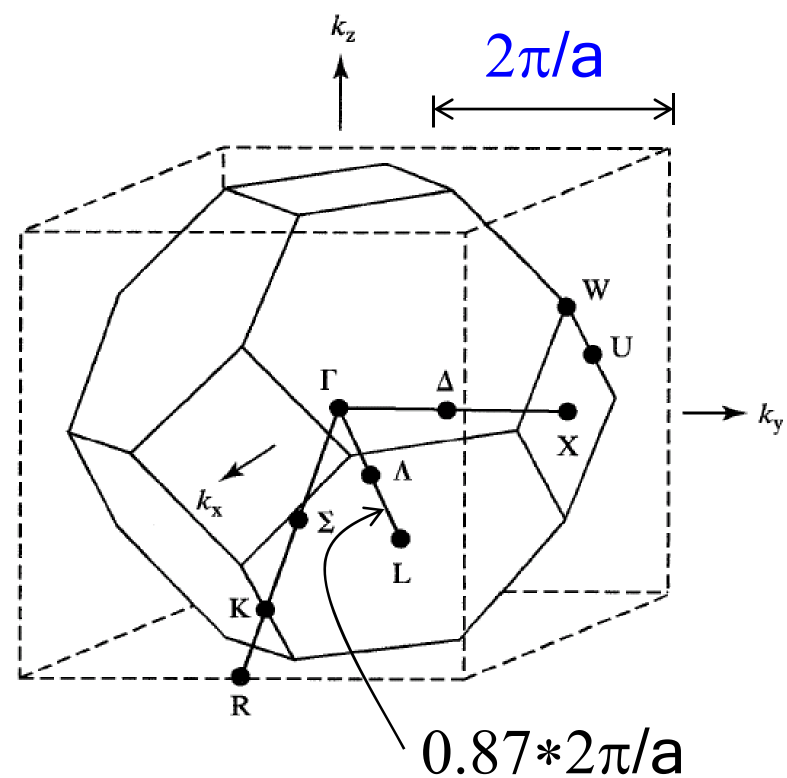
Follow W-S algorithm, but now for reciprocal lattice

Brillouin Zone in *Real* FCC Lattices …

Real Space FCC
(for Si, Ge, GaAs)

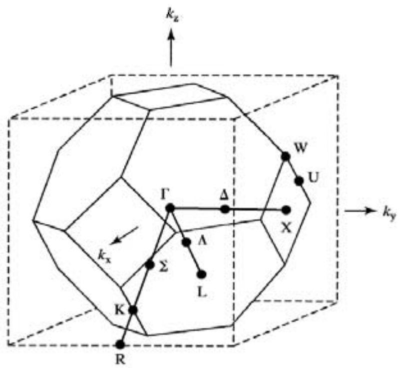


Reciprocal Lattice



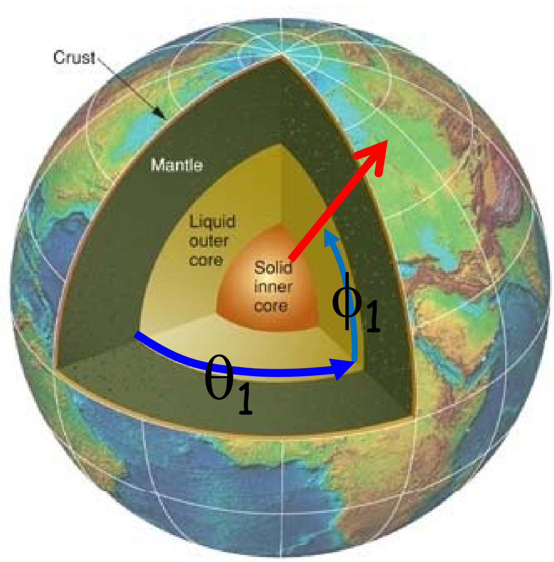
Note unlike cubic lattice, zone edge is not at π/a

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

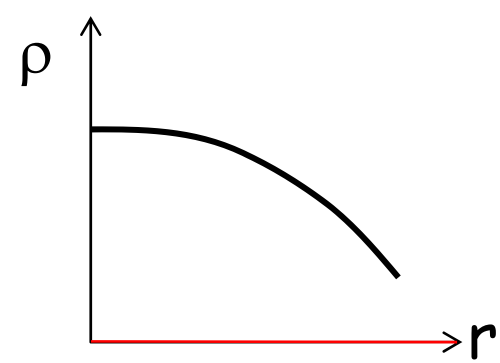


Density (x,y,z)

4D information

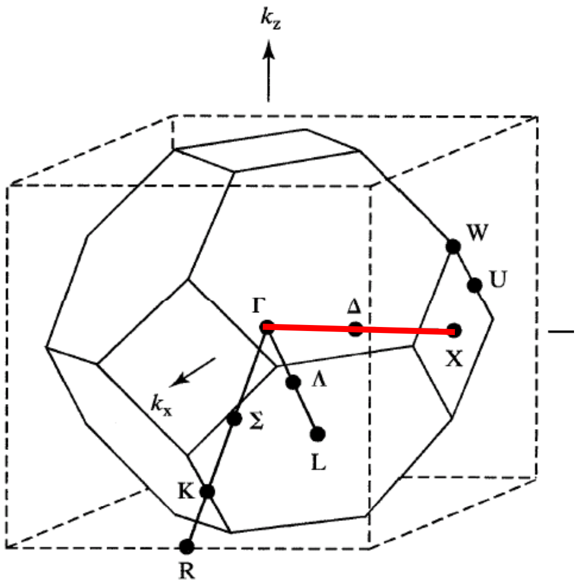


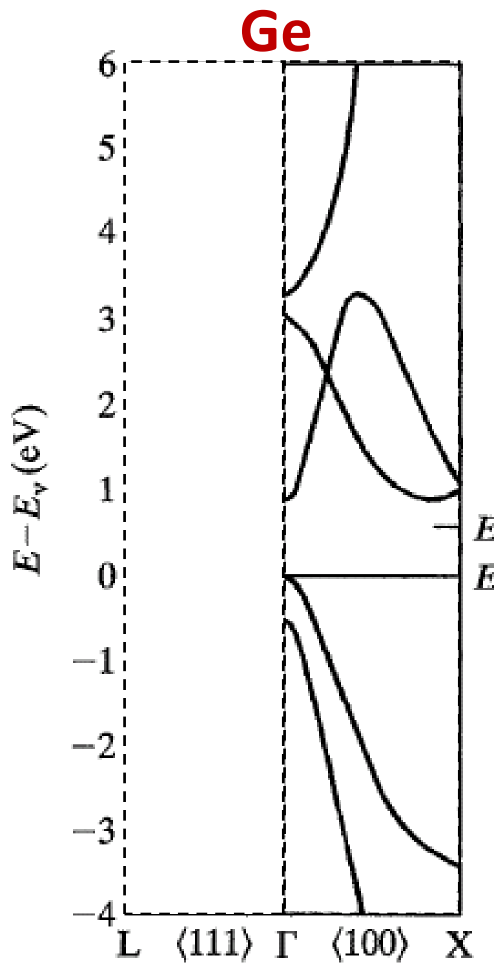
Cut along (θ_1, ϕ_1) …



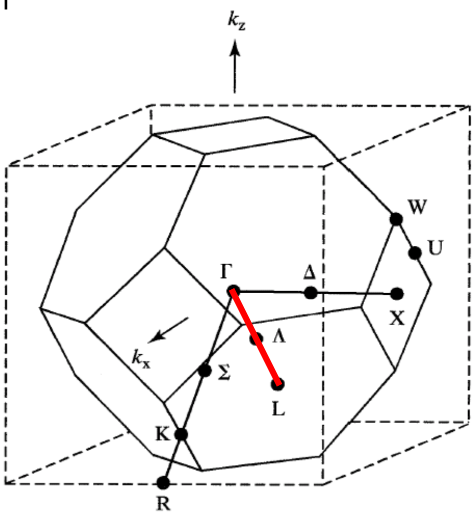
A series of line-sections can Represent the 4D info in 2D plots

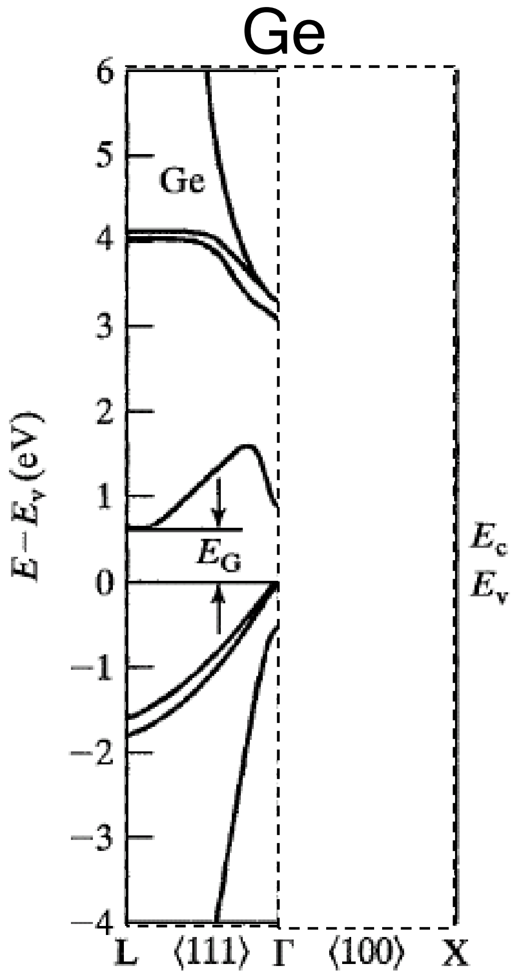
E-k along Γ-X Direction



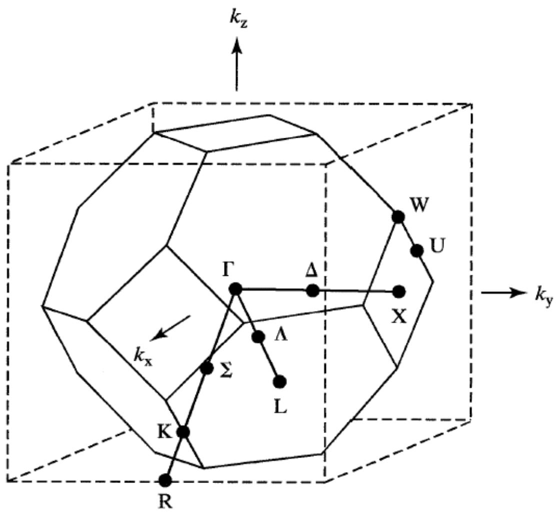


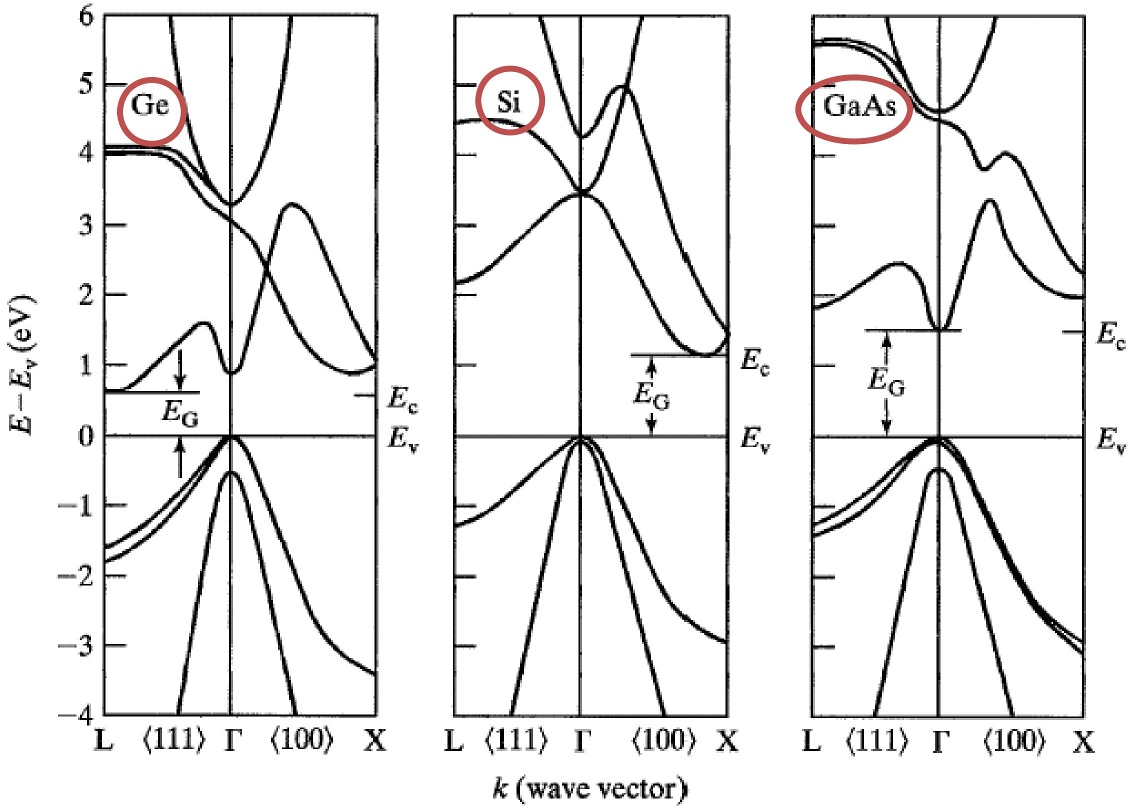
E-k along Γ-L direction





E-k Diagram

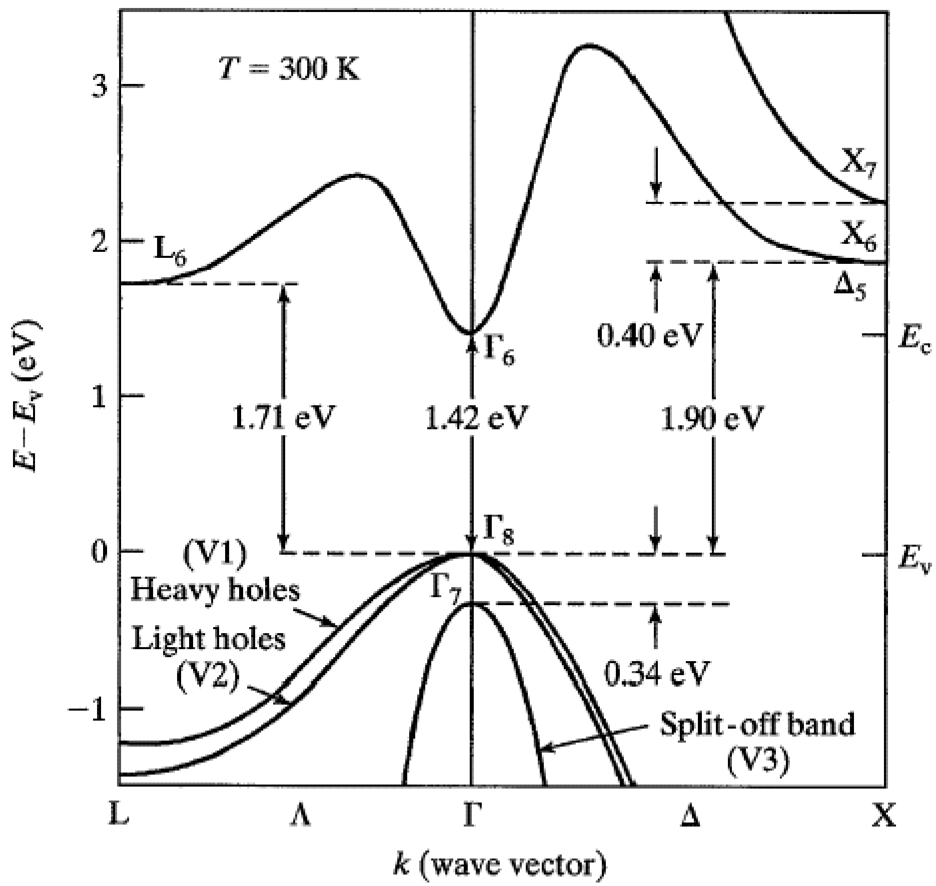




- 3 valence bands (light hole, heavy hole, split-off) valence bands near k=0 is essentially $E \sim k^2$

- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: Γ valleys)

E-k diagram for GaAs

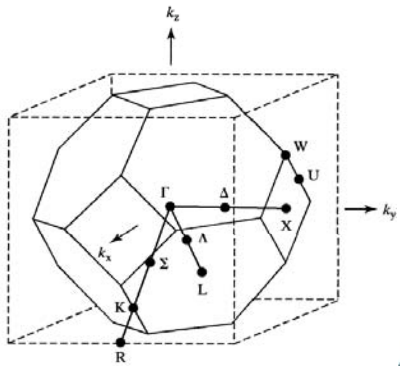


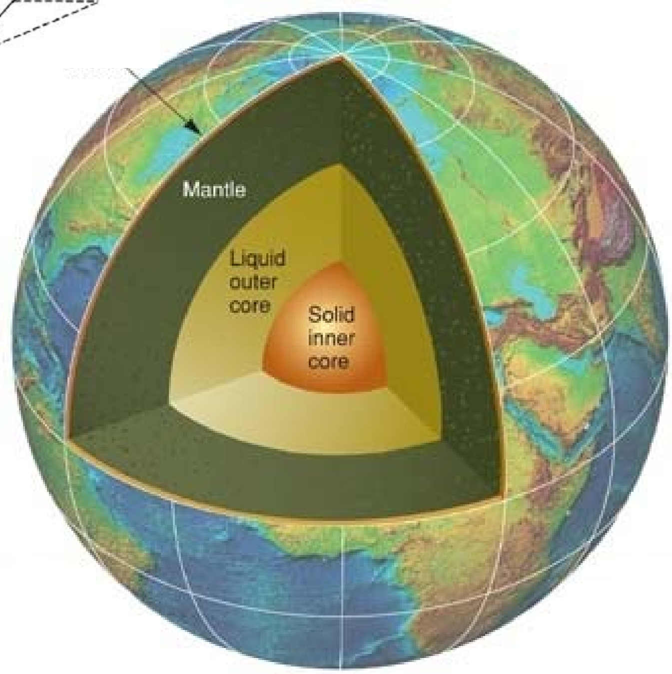
Direct bandgap material

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

Has important implications
For transport

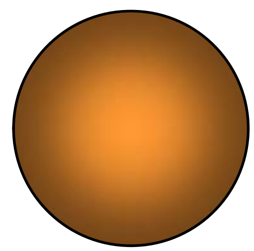
Analogy for E-k Diagram



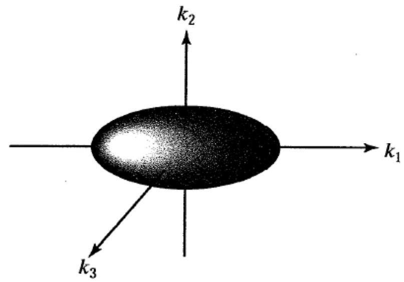


Density (x,y,z)

Contours of density ….

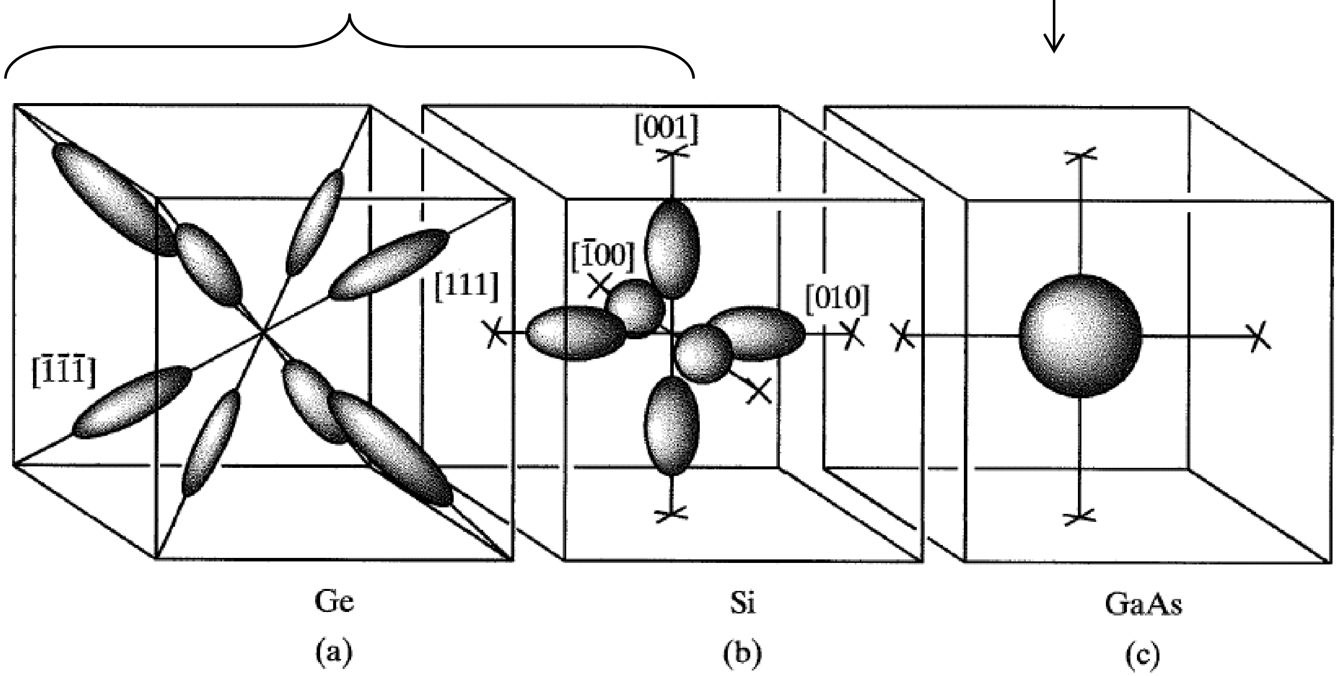


Constant-E surface for Conduction Band



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

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



Constant E-surface …

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

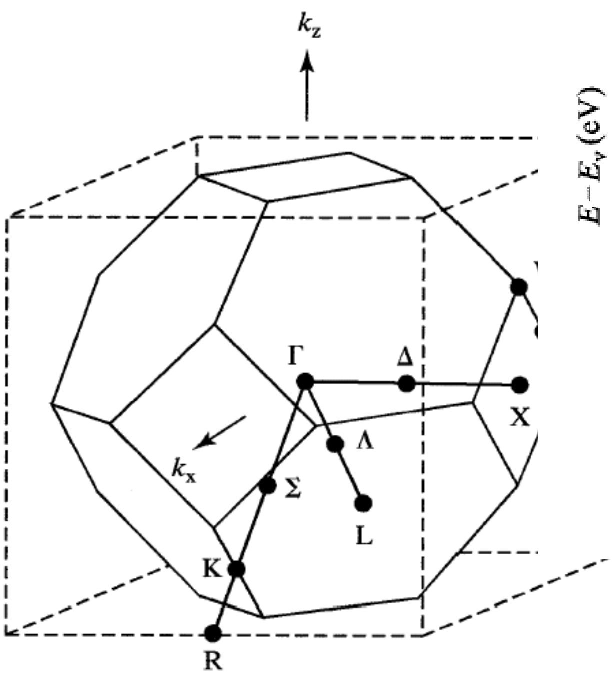
$$E = E_c + A(k_1^2 + k_2^2 + k_3^2)$$

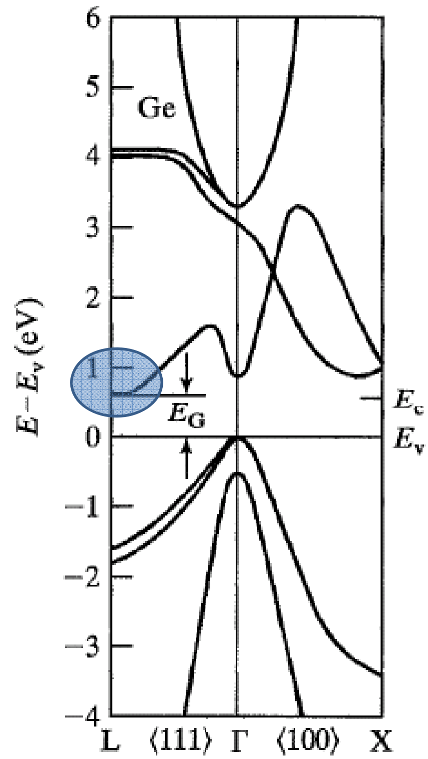
$$\frac{1}{m_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

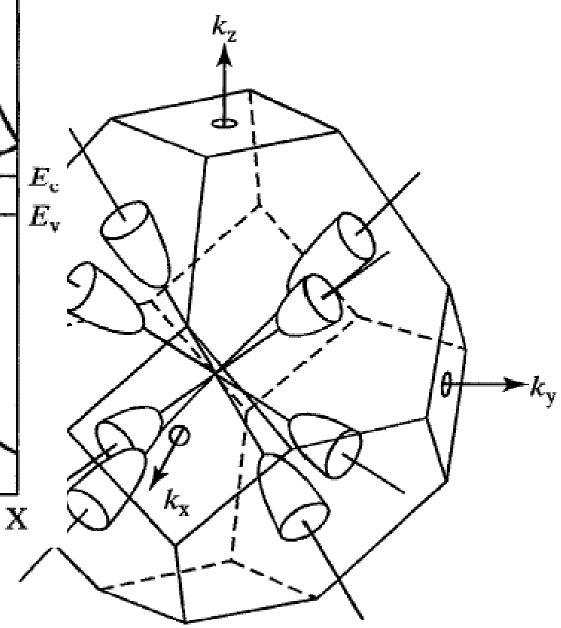
$$\frac{1}{m_{11}} = \frac{2A}{\hbar^2};\quad \frac{1}{m_{22}} = \frac{1}{m_{33}} = \frac{2B}{\hbar^2};\quad \frac{1}{m_{ij}(i \neq j)} = 0$$

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

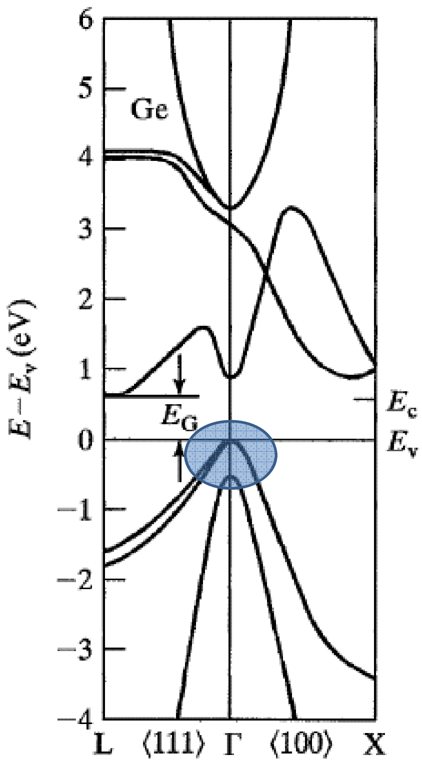
Four valleys inside BZ for Germanium

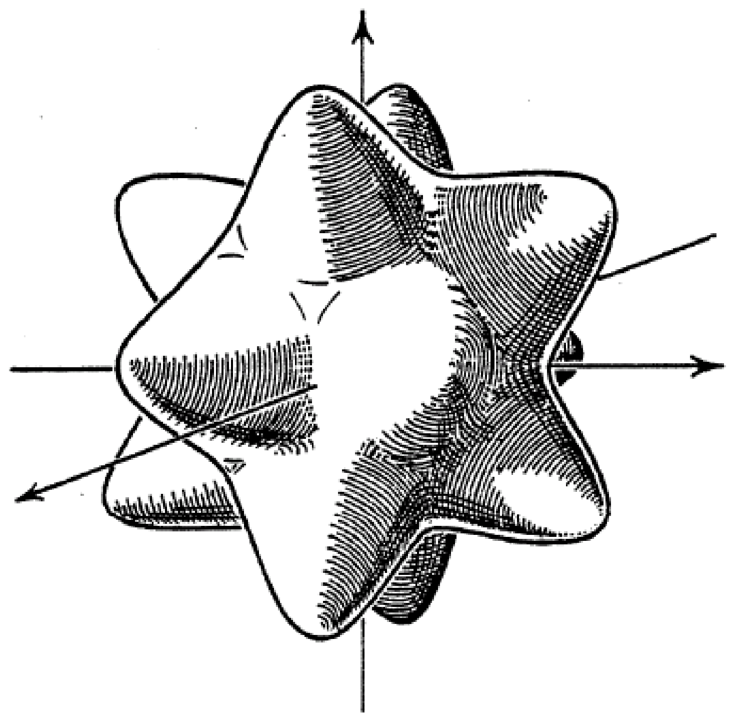






Constant E-surface for Valence Band





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

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

Outline

1) E-k diagram/constant energy surfaces in 3D solids

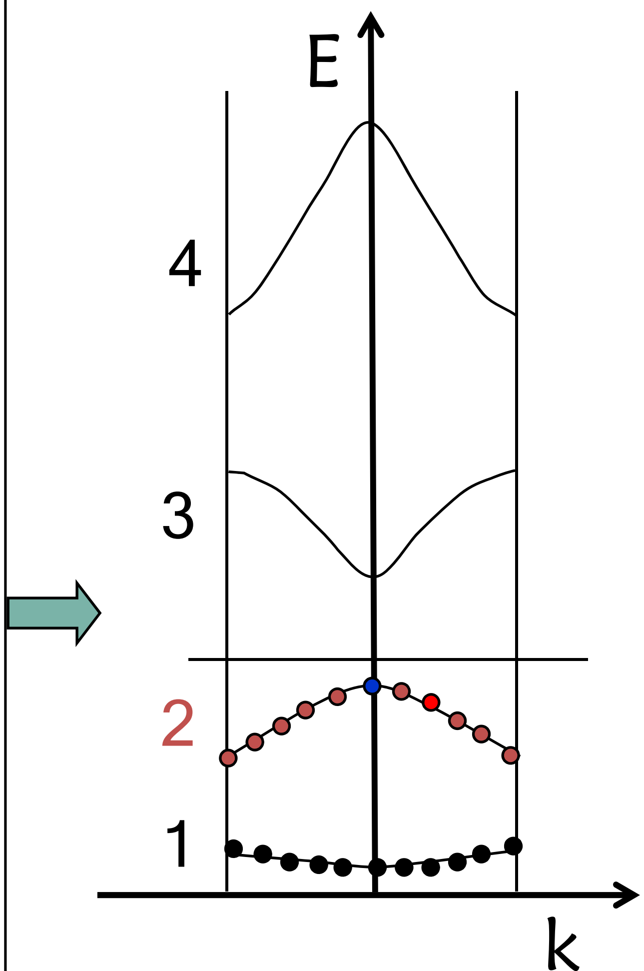
2) **Characterization of E-k diagram: *Bandgap***

3) Characterization of E-k diagram: Effective Mass

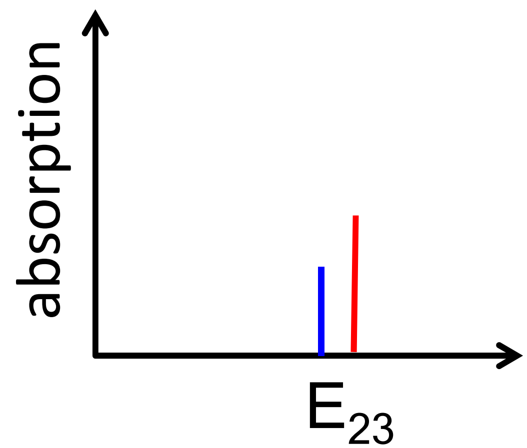
4) Conclusions

Reference: Vol. 6, Ch. 3 (pages 71-77)

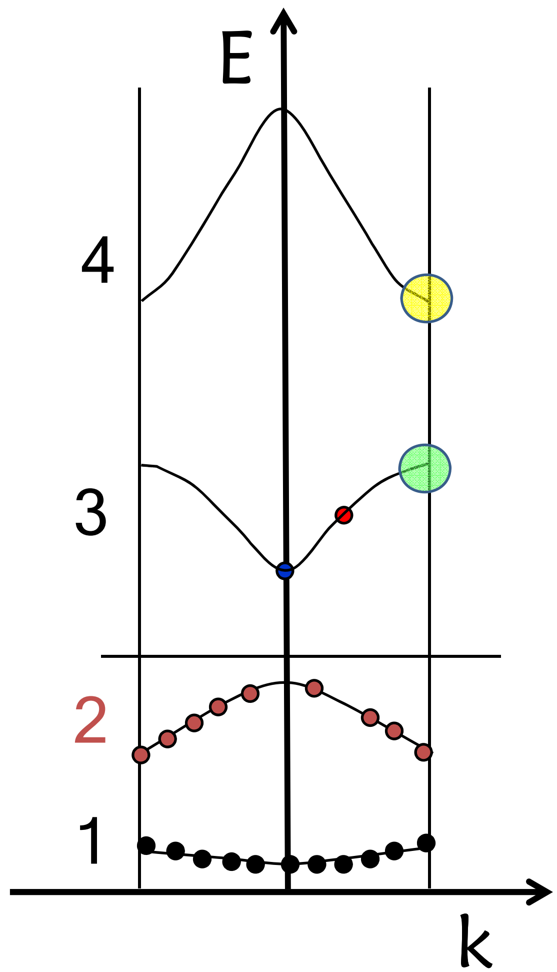
Measurement of Band Gap

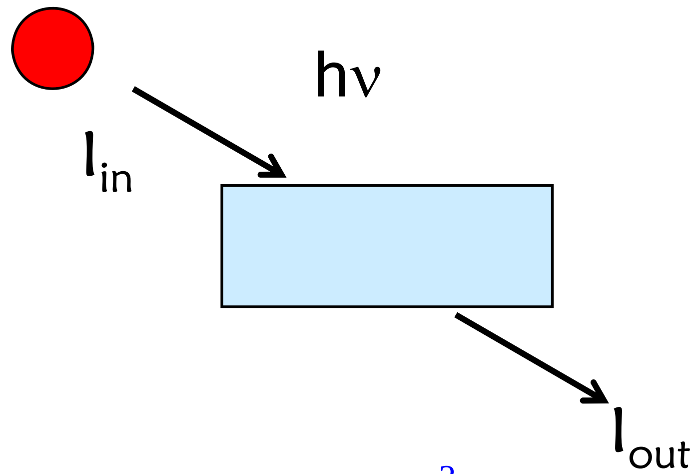


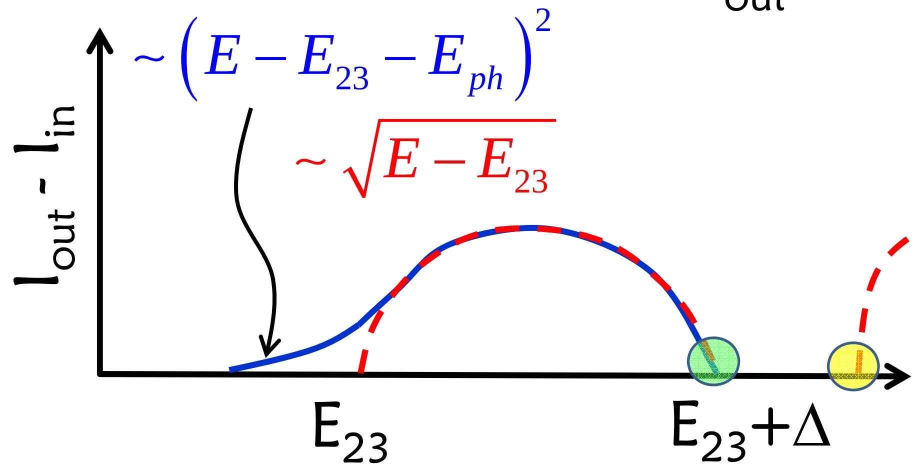
Photons are only absorbed between bands that have filled and empty states



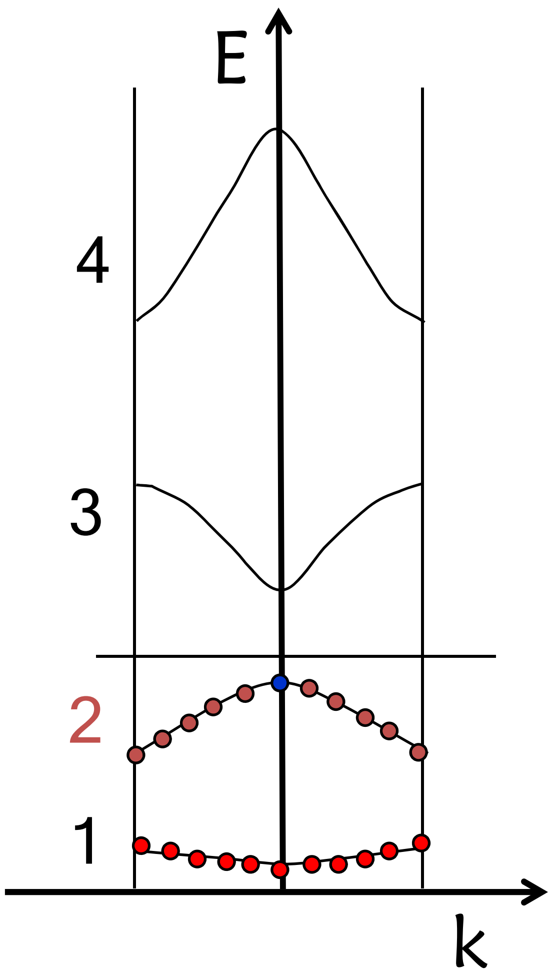
Measurement of Energy Gap

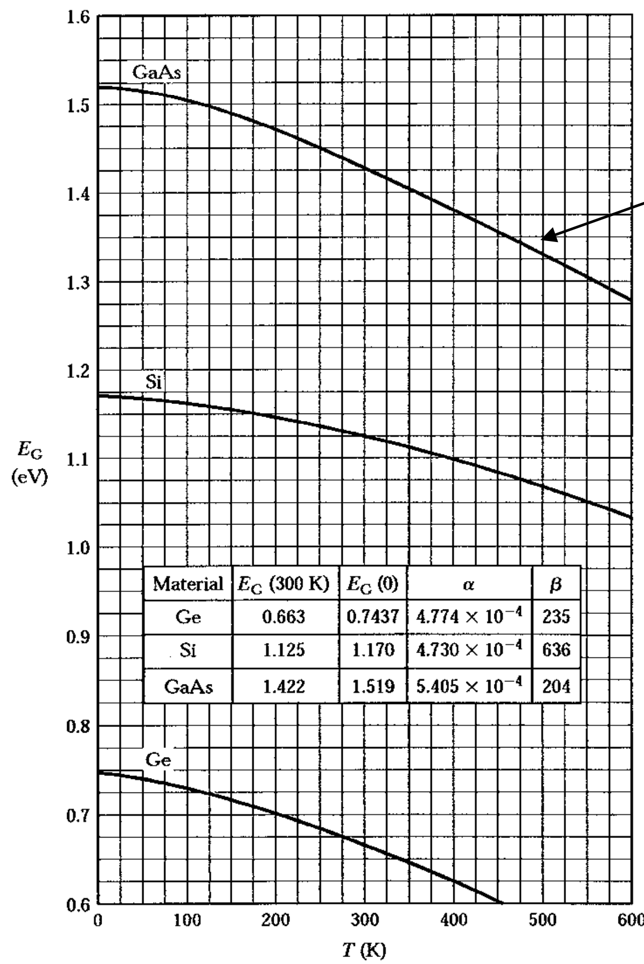






Temperature-dependent Band Gap





Material	E_G (300 K)	E_G (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

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

Outline

1) E-k diagram/constant energy surfaces in 3D solids

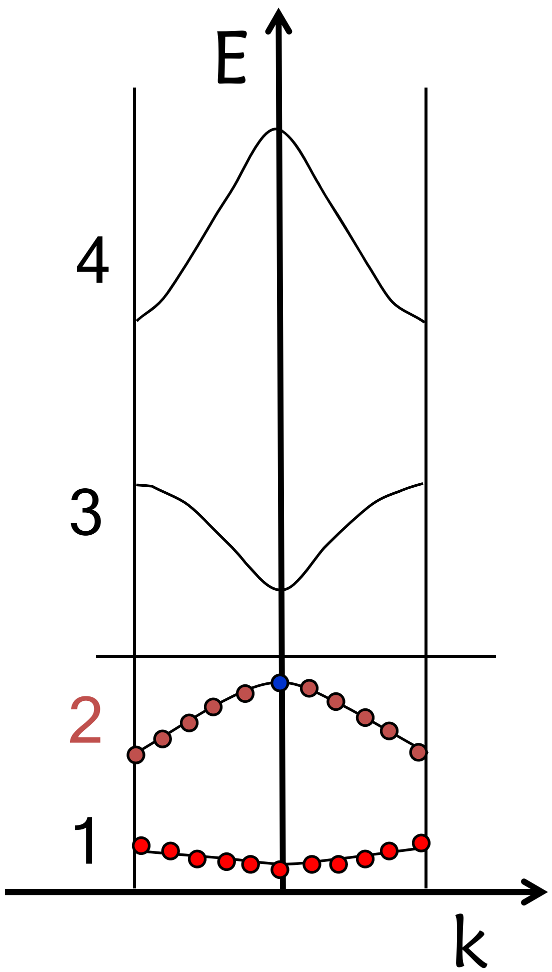
2) Characterization of E-k diagram: Bandgap

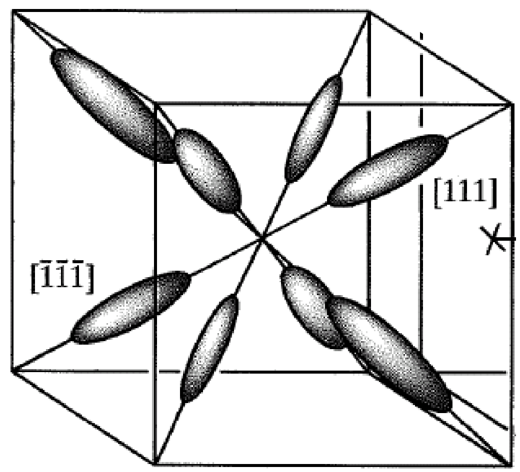
3) **Characterization of E-k diagram: Effective Mass**

4) Conclusions

Reference: Vol. 6, Ch. 3 (pages 71-77)

Measurement of Effective Mass

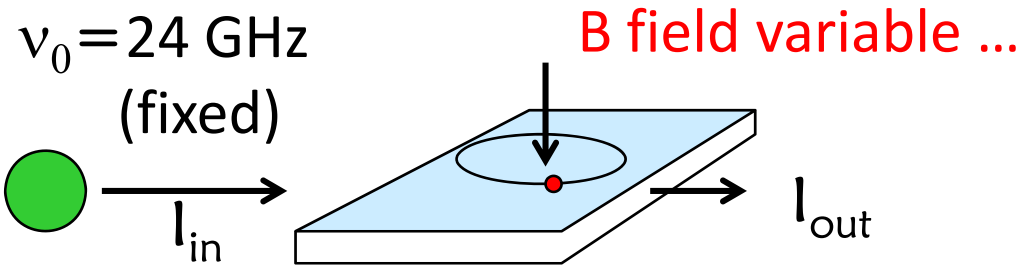


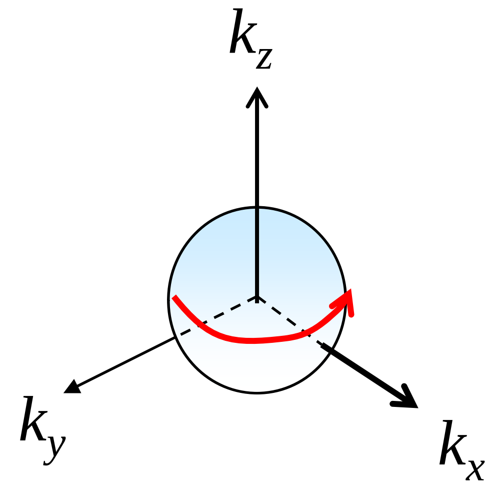


Ge

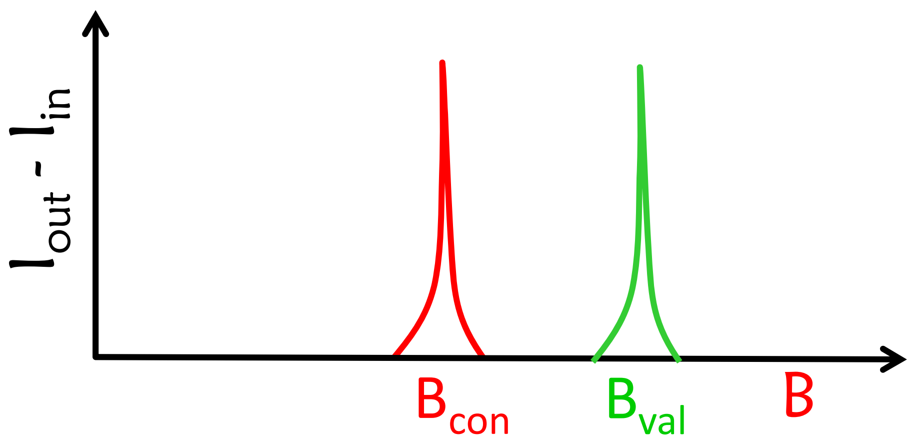
(a)

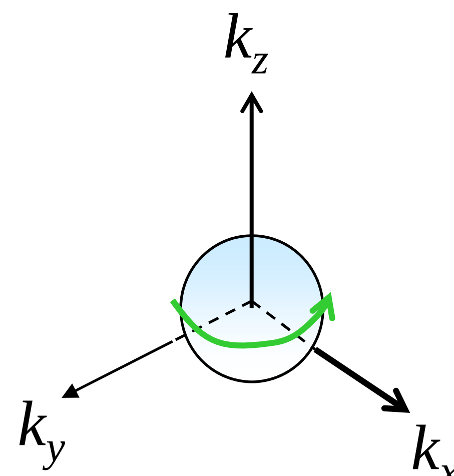
Measurement of Effective Mass





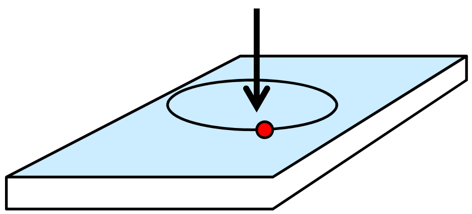
$$\nu_0 = \frac{qB_0}{2\pi m^*} \qquad m^* = \frac{qB_0}{2\pi \nu_0}$$





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 …



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

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

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

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

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

Conclusions

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) Experimental measurements are key to making sure that the theoretical calculations are correct. We will discuss them in the next class.