

## Section 10

### Bandstructure in Real Materials (Si, Ge, GaAs)

#### 10.2 Constant Energy Surfaces - Effective Mass Tensor

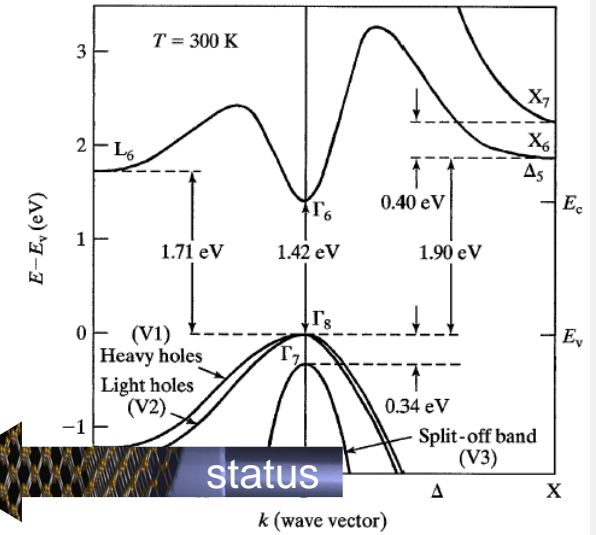
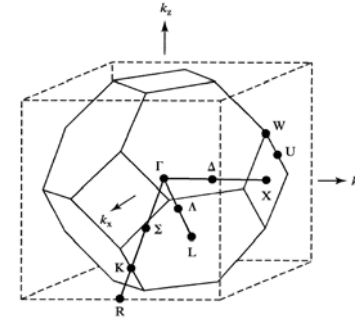
Gerhard Klimeck  
[gekco@purdue.edu](mailto:gekco@purdue.edu)



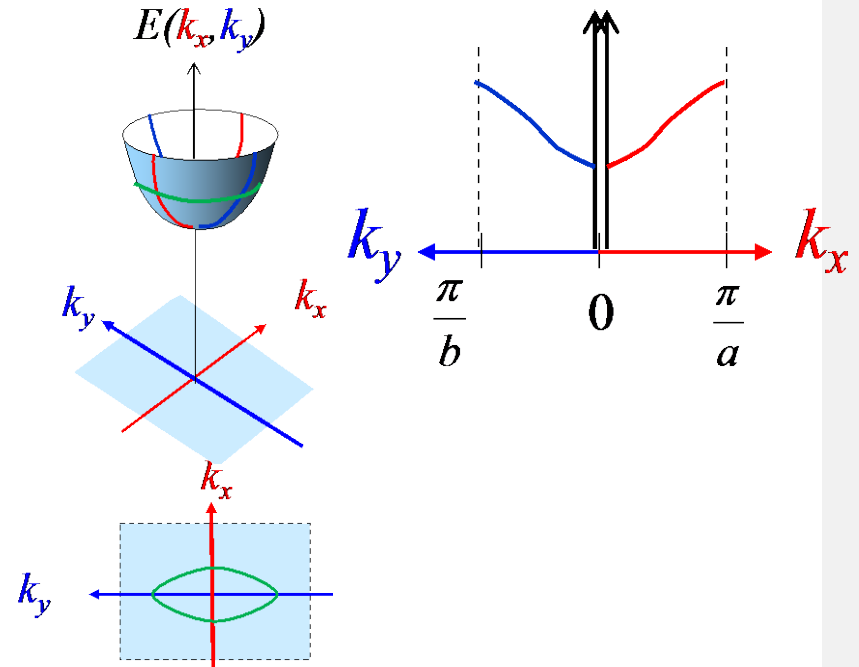
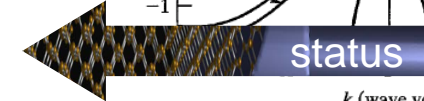
School of Electrical and  
Computer Engineering

# Section 10 Bandstructure in Real Materials (Si, Ge, GaAs)

• 10.1 E(k) diagrams in specific crystal directions



• 10.2 Constant Energy Surfaces – Effective Mass Tensor



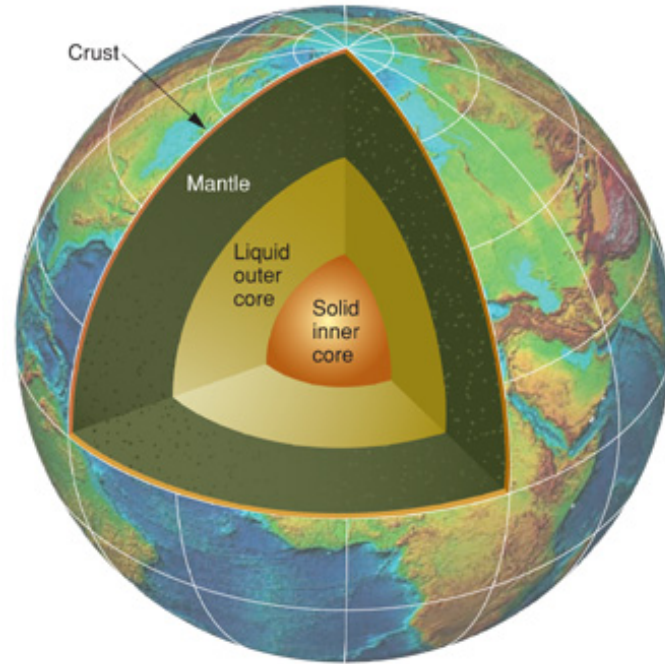
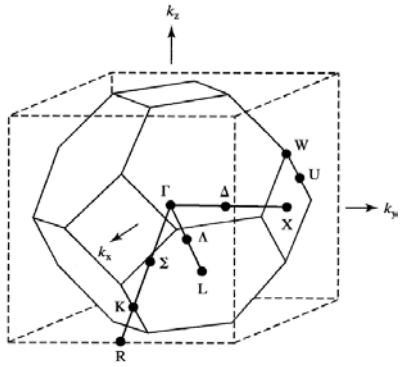
• 10.3 Density of States Effective Mass

One Video Segment

One Video Segment

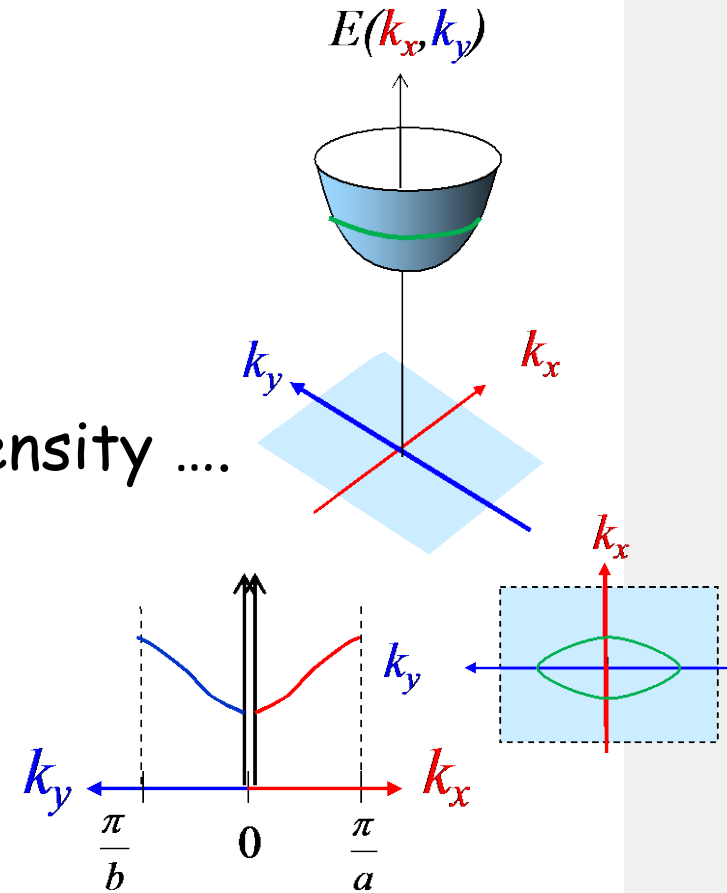
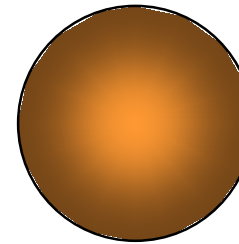
One Video Segment

# Analogy for E-k Diagram

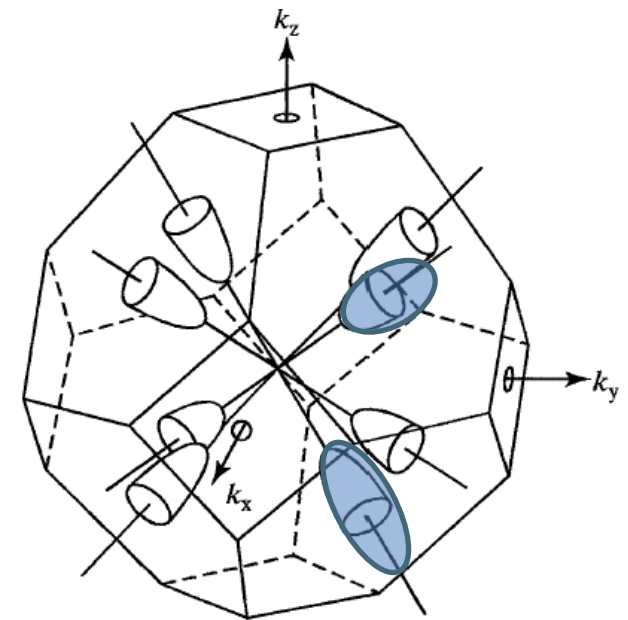
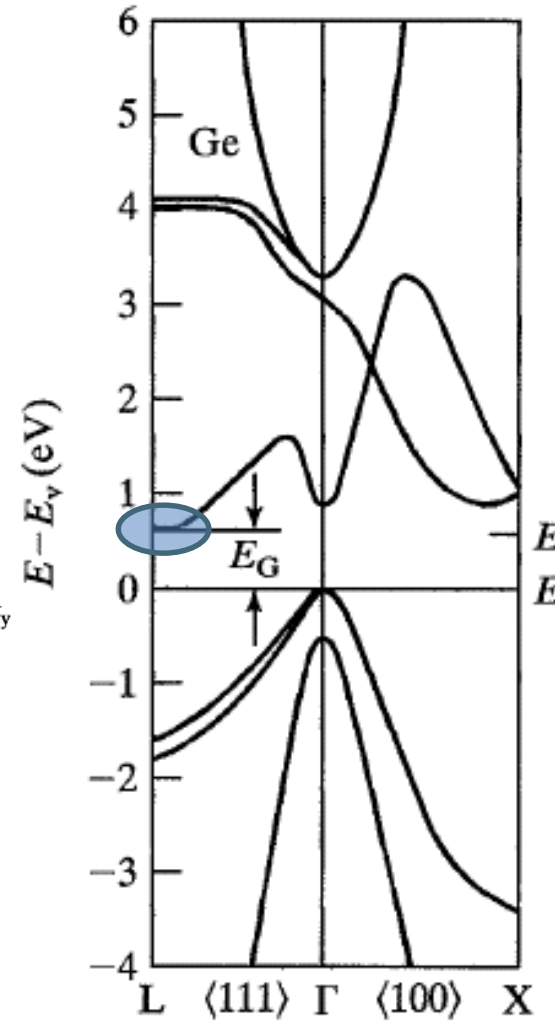
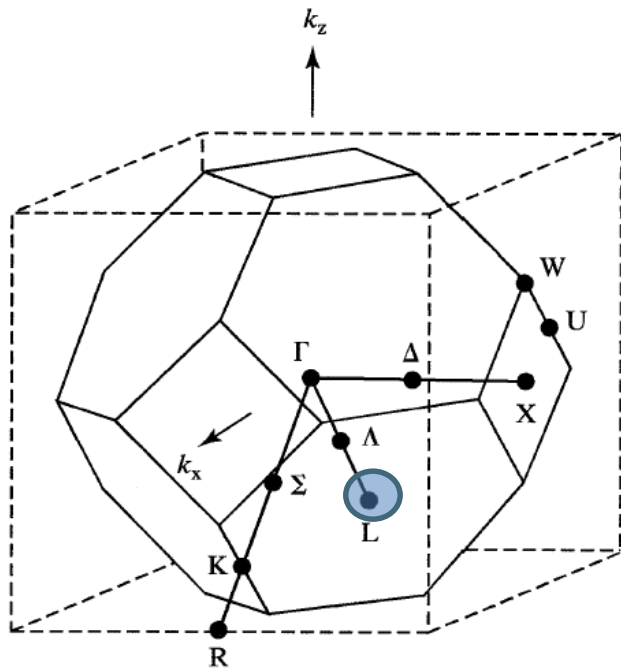


Density (x,y,z)

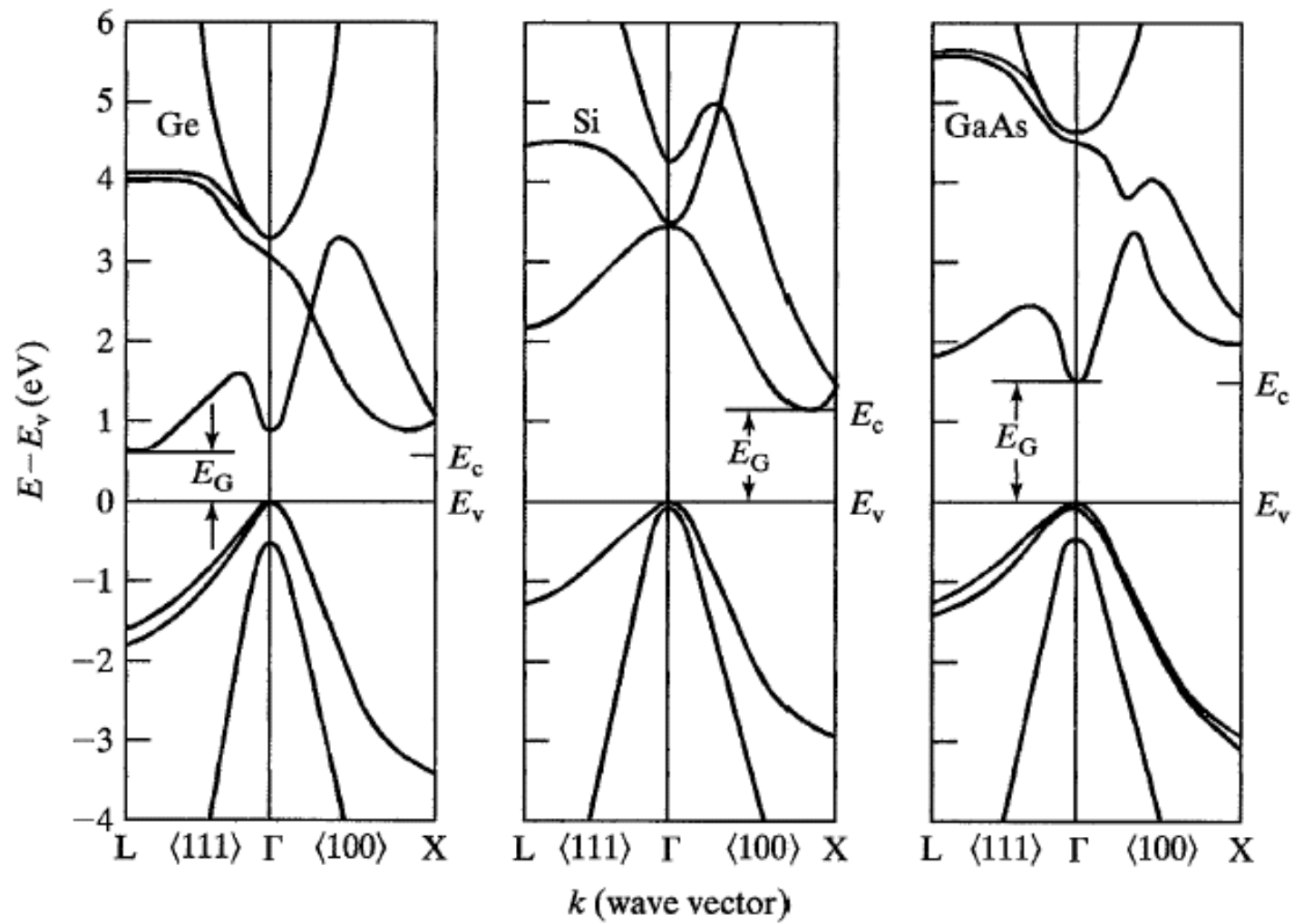
Contours of density ....



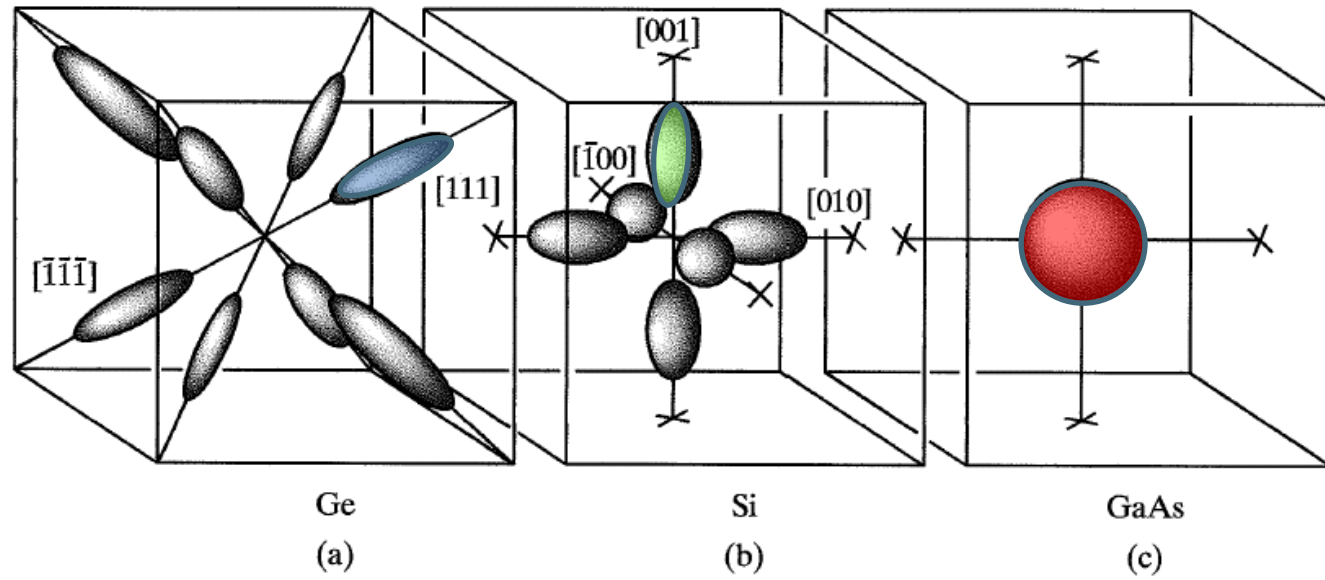
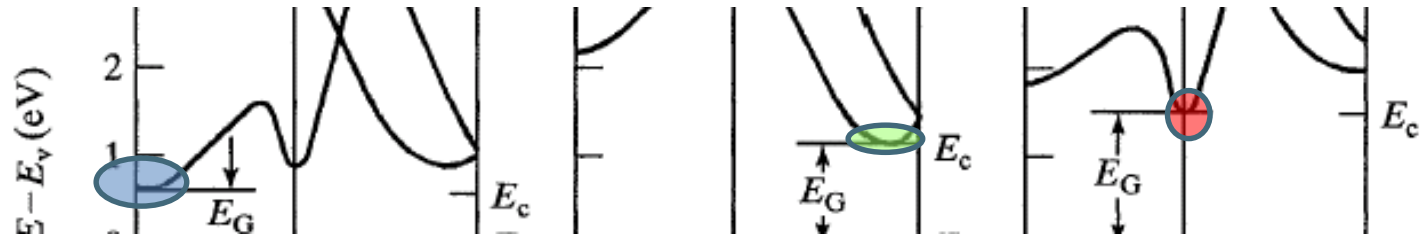
# Four valleys (8 halves) inside BZ for Germanium



# Constant-E surface for Conduction Band

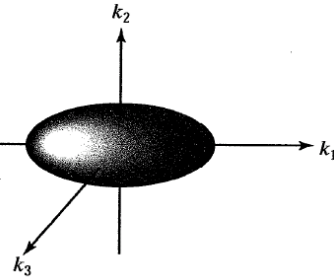


# Constant-E surface for Conduction Band

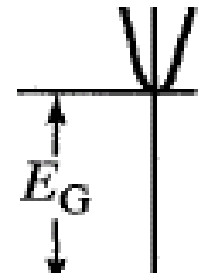
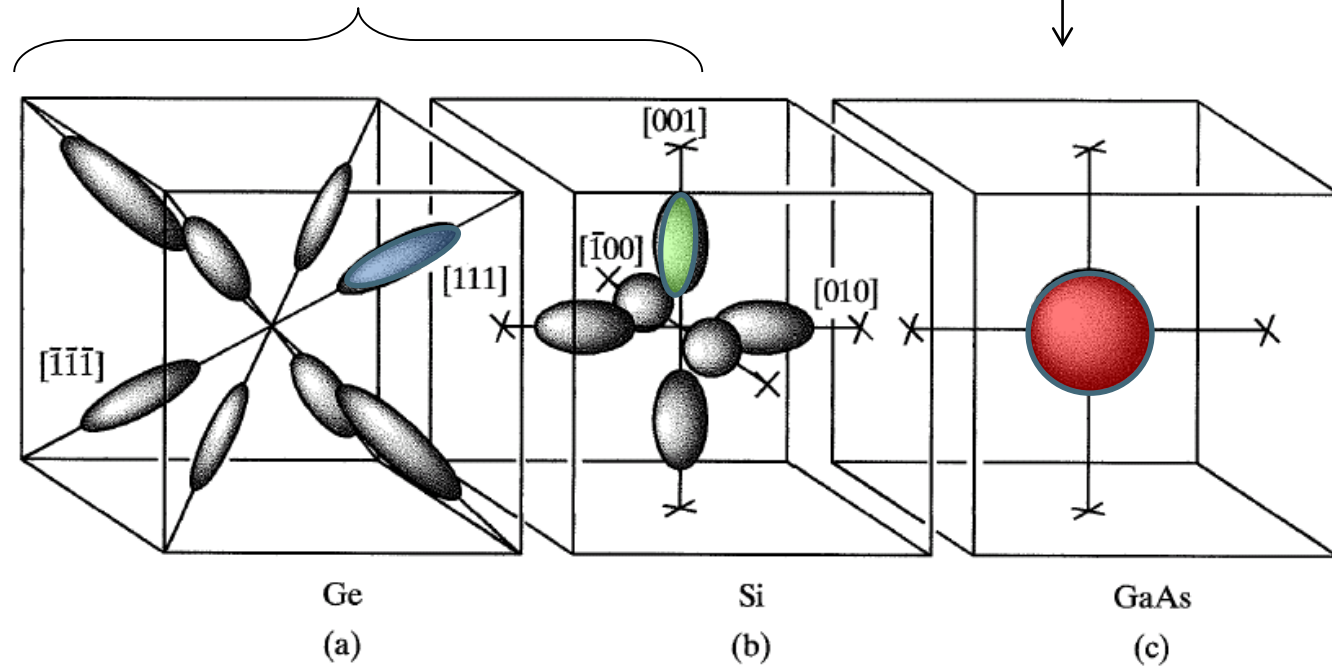
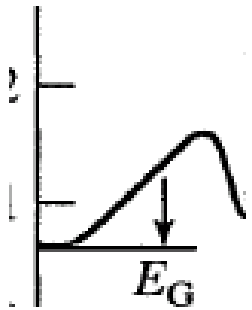


# Constant-E surface for Conduction Band

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



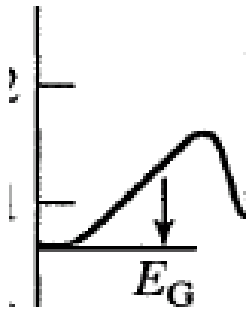
$$E = E_c + A(k_1^2 + k_2^2 + k_3^2)$$



# Constant E-surface and Effective Mass Tensor

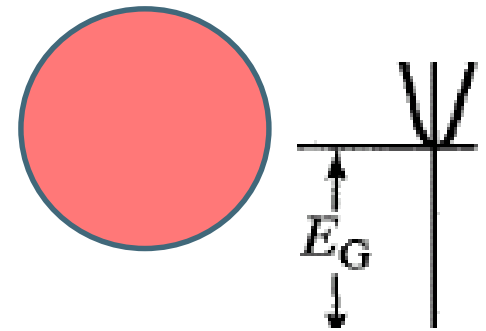
$$E = E_c + Ak_1^2 + B(k_2^2 + k_3^2)$$

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



Ge: 8 valleys  
Si: 6 valleys

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



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

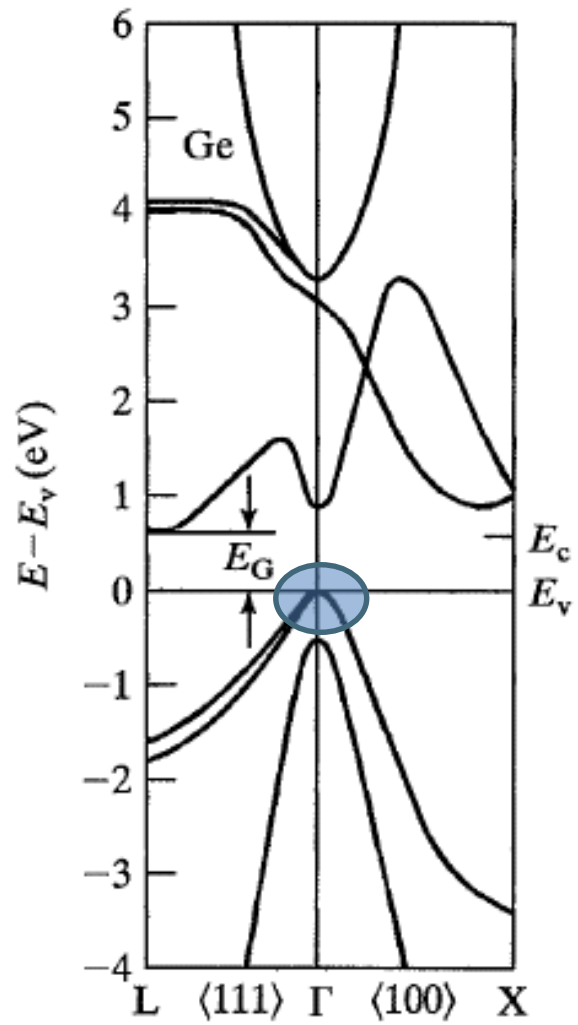
1 heavy mass  
2 light masses

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

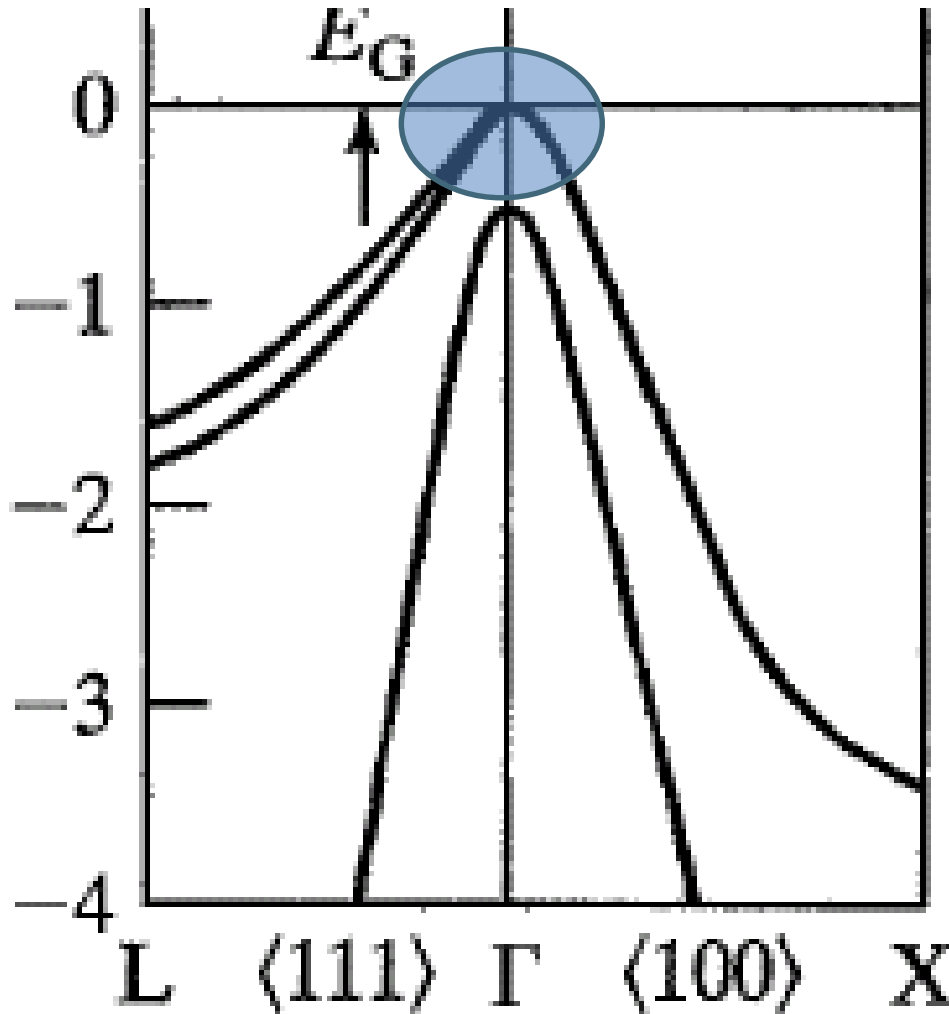
Offdiagonal Elements=0  
=> Force and movement aligned



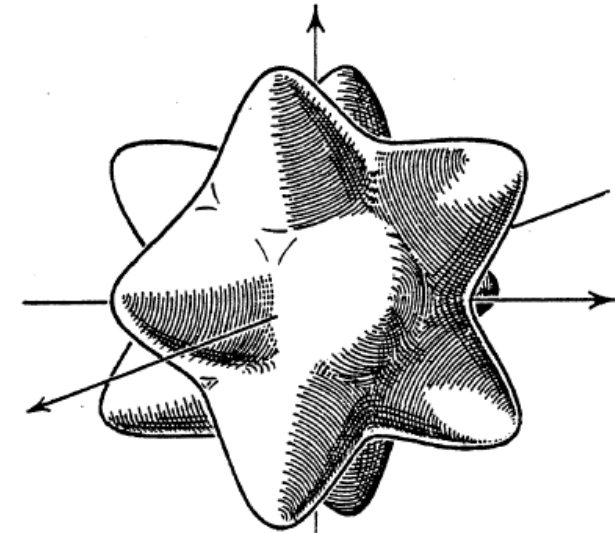
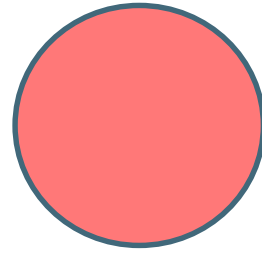
# Constant E-surface for Valence Band



# Constant E-surface for Valence Band



$E_c$   
 $E_v$



3 bands:  
 HH – Heavy Hole  
 LH – Light Hole  
 SO – Split-off band

HH and LH are NOT  
 Isotropic  
 => NOT spheres  
 => strong spatial variations

Rotated substrate  
 technology at TI  
 Robert C. Bowen  
 Enhanced PMOS

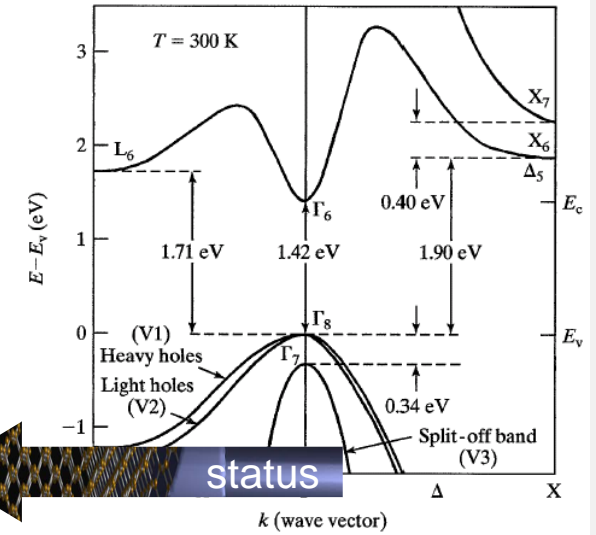
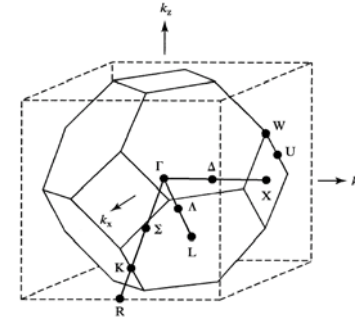
$$E = E_v - Ak^2 \mp \sqrt{[B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)]}$$

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

# Section 10

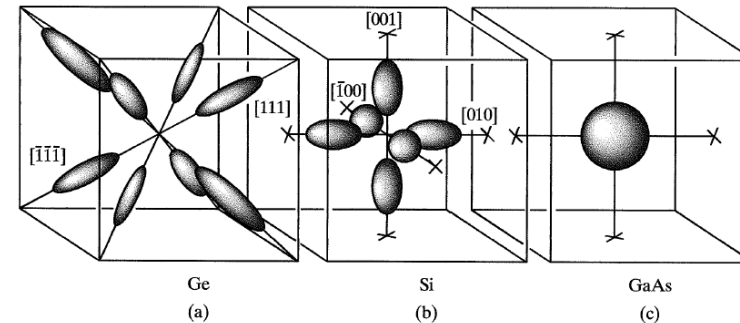
## Bandstructure in Real Materials (Si, Ge, GaAs)

- 10.1 E(k) diagrams in specific crystal directions

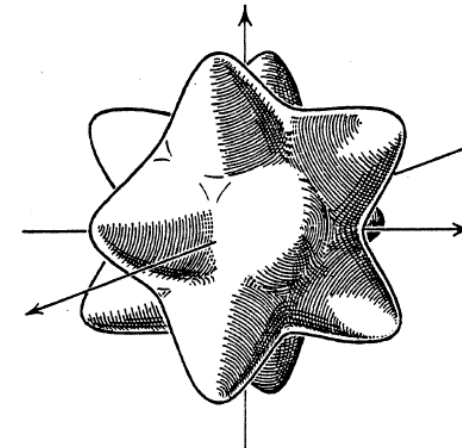


- 10.2 Constant Energy Surfaces – Effective Mass Tensor

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



- 10.3 Density of States Effective Mass



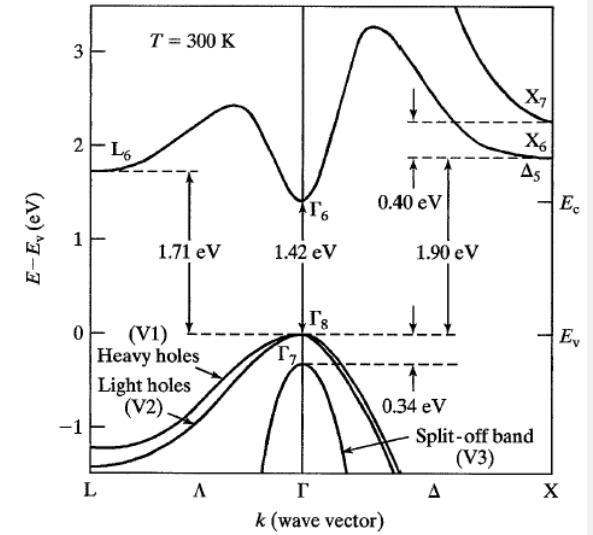
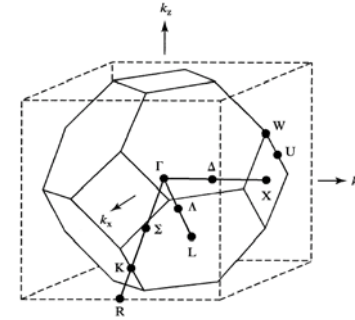
One Video Segment

One Video Segment

One Video Segment

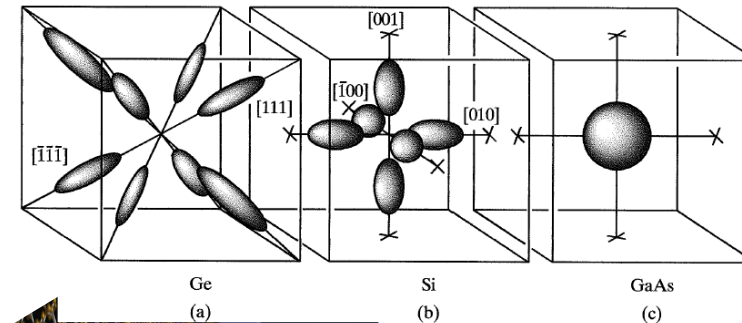
# Section 10 Bandstructure in Real Materials (Si, Ge, GaAs)

- 10.1 E(k) diagrams in specific crystal directions

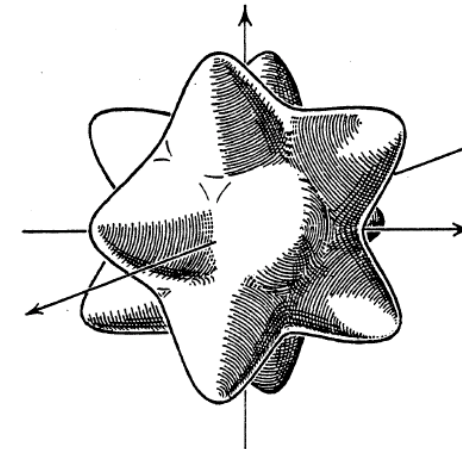
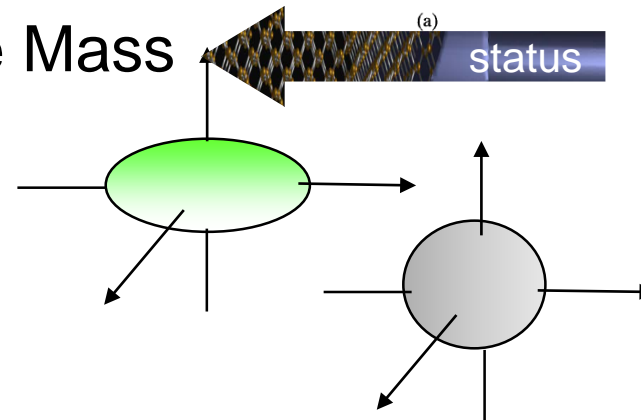


- 10.2 Constant Energy Surfaces – Effective Mass Tensor

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



- 10.3 Density of States Effective Mass



# Section 10

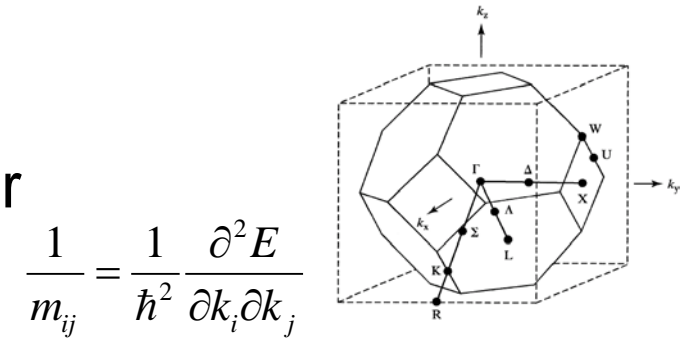
## Bandstructure in Real Materials (Si, Ge, GaAs)

Video

Video

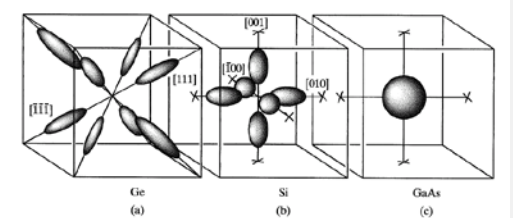
Video

- 10.1 E(k) diagrams in specific crystal directions
- 10.2 Constant Energy Surfaces – Effective Mass Tensor
- 10.3 Density of States Effective Mass



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

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



- 1) E-k diagrams emerge from the solution of Schrödinger's Eq.
- 2) E-k diagrams at which energy an electron with a specific crystal momentum **can** reside.
- 3) E-k diagrams depend on the underlying crystal symmetry
- 4) Only a fraction of the available states are occupied. The number of available states change with energy.
- 5) DOS of g(E) describes the number of available states in a small energy window around energy E
- 6) DOS is an important and useful characteristic of a material

