VI. Features in Semiconductor Energy Bands

- Look at some features in semiconductor bands
- Description of Key Parts of semiconductor bands
- Effective Mass Approximation
- Velocity of Bloch state and Effective Mass
- Momentum Matrix Elements

A. Spin-Orbit Interaction Effect

- Observed in atomic spectrum: Fine structure

  splitting of spectral lines (no external field)

Idea: $\vec{B}_{int}$ due to electron's motion ($\propto \vec{L}$ and thus $\vec{r} \times \vec{p}$)

$\sim (\vec{\nabla} V \times \vec{p})$

in a potential energy function

[e.g. $V(\vec{r})$ in atoms, $V(\vec{r})$ in solids]

$\vec{p}$: electron's momentum

Electron has spin angular momentum $\vec{S}$ $\left(\vec{S} = \frac{\hbar}{2}\vec{\sigma}\right)$

$\vec{\sigma}$: Pauli matrices

$$\vec{\mu}_s = \frac{-e}{m_e}\vec{S}$$

$\vec{\mu}_s$: spin magnetic dipole moment

$\therefore$ Interaction energy $= -\vec{\mu}_s \cdot \vec{B}_{int} \propto \vec{S} \cdot \vec{L} \propto \vec{\sigma} \cdot (\vec{\nabla} V \times \vec{p})$

Let the formula talk...

$$H_{so} = \frac{\hbar}{4m^2c^2}\,\vec{\sigma}\cdot\left(\vec{\nabla}V \times \vec{p}\right) \qquad (1)$$

① when an electron moves...

② ... perpendicularly to a gradient of a potential energy landscape,

③ there is a (an effective) magnetic field that interacts with the electron's spin

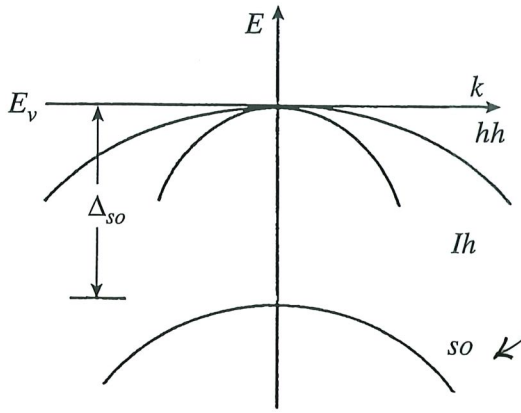
$\vec{p}$: electron's momentum (so "moves")

$\vec{\sigma}$: Pauli spin matrix $\vec{\sigma} = \sigma_x\hat{x} + \sigma_y\hat{y} + \sigma_z\hat{z}$ (electron's spin)

($\sigma_x, \sigma_y, \sigma_z$: Pauli matrices)

- Should include H_{so} and other relativistic corrections into Band Problem
- What to expect?
  - Not important for states of strongly s-character (e.g. conduction band minimum)
  - More important for states of strongly p-character (e.g. top of VB's)

[$\ell = 1$ atomic states]



Valence bands near the Brillouin zone center for diamond structure semiconductors with spin–orbit splitting Δ_{so}. The bands shown are the heavy hole (*hh*), light hole (*lh*), and split-off (*so*) bands. Each band is doubly degenerate.

← Features near top of Valence bands due to H_{so} (Schematic)

- Split off VB

p-states: 6 p-states (with spin)

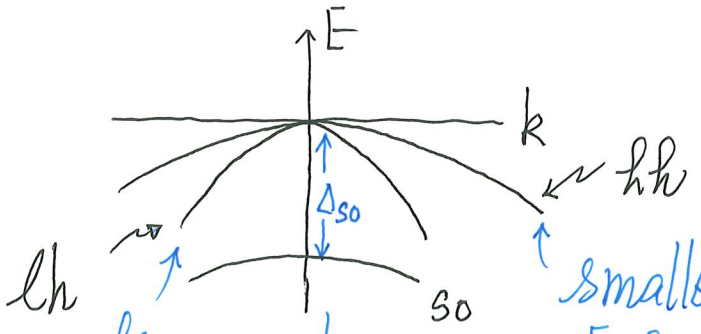
atomic: $\ell = 1,\ s = 1/2 \Rightarrow \begin{cases} j = 3/2 & (m_j = 3/2, 1/2, -1/2, -3/2) \\ j = 1/2 & (m_j = 1/2, -1/2) \end{cases}$

↓

these states form split off VB

"heavy hole" (hh)

"light hole" (lh)



bigger curvature

[smaller (but negative) electron effective mass]

smaller curvature

[bigger (but negative) electron effective mass]

e.g. Ge: $\Delta_{so} \cong 0.3\,eV$ (c.f. $E_{gap} \sim 0.74\,eV$)

Ge: heavier; indirect

Diamond: $\Delta_{so} \approx 0.006\,eV$ (c.f. $E_{gap} \sim 5.4\,eV$)

(carbon): light atoms; insulator

GaAs: $\Delta_{so} \approx 0.34\,eV$ (c.f. $E_{gap} \sim 1.52\,eV$)

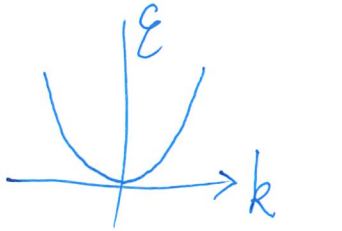
- Heavy atoms, stronger $\vec{B}_{int}$, bigger Δ_{so}

Recall: Free electron ($V(\vec{r}) = 0$)

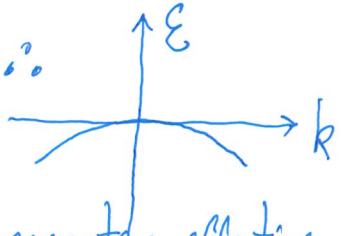
$$\mathcal{E}(\vec{k}) = \underbrace{\frac{\hbar^2 k^2}{2m_e}}_{\sim k^2 \text{ (quadratic)}} ; \quad \psi_{\vec{k}} \sim e^{i\vec{k}\cdot\vec{r}}$$

$\sim m_e$ gives curvature

But m_e (real electron) > 0,



$\therefore$

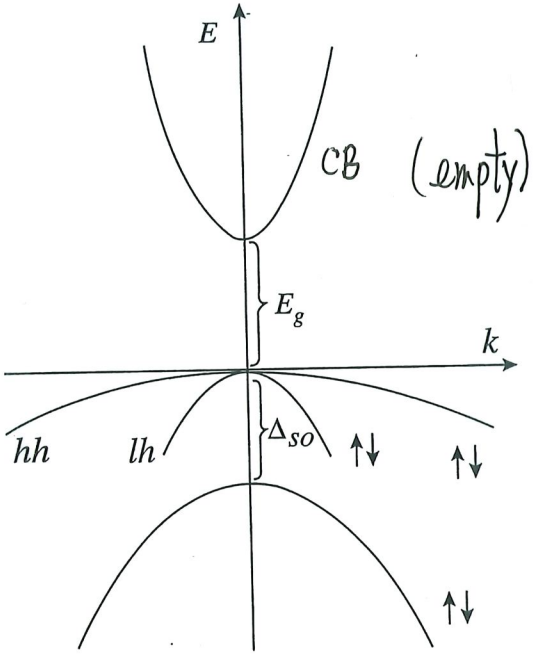


negative effective electron mass

A good Model of Band Structure to keep in mind (4-Band Model)

← just a small part of → 1st B.Z.

↑ more empty CB's of higher energy (usually irrelevant)



Heavy hole (*hh*), light hole (*lh*), and split-off (*so*) energy bands for diamond structure semiconductors. The Kramers degeneracy is indicated by the up and down arrows.

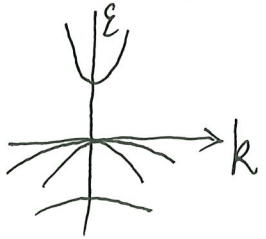
most important group of bands for properties of semiconductors

↓ more completely filled bands from core states (irrelevant)

Even for Indirect gap materials

(Si, Ge)

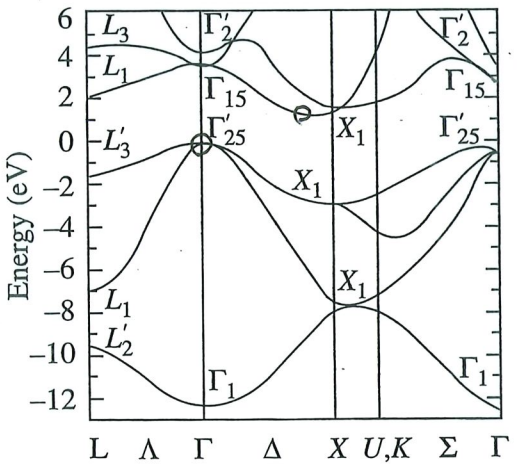
the valence bands structure (VB's) is still determined predominately by



near the top of VB's

most important part of VB's

B. Some Band structures

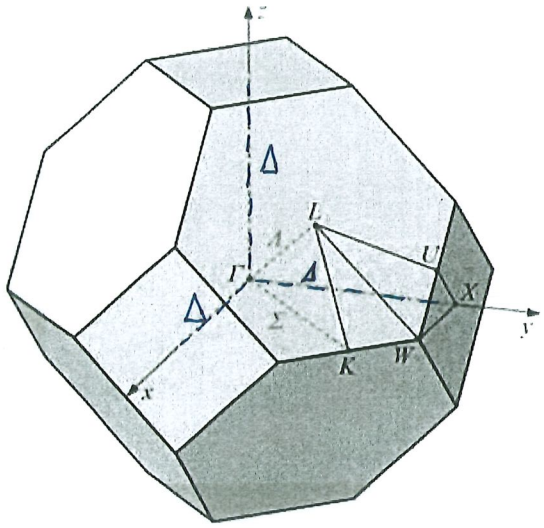


Band structure of Si (after Chelikowsky and Cohen 1976).

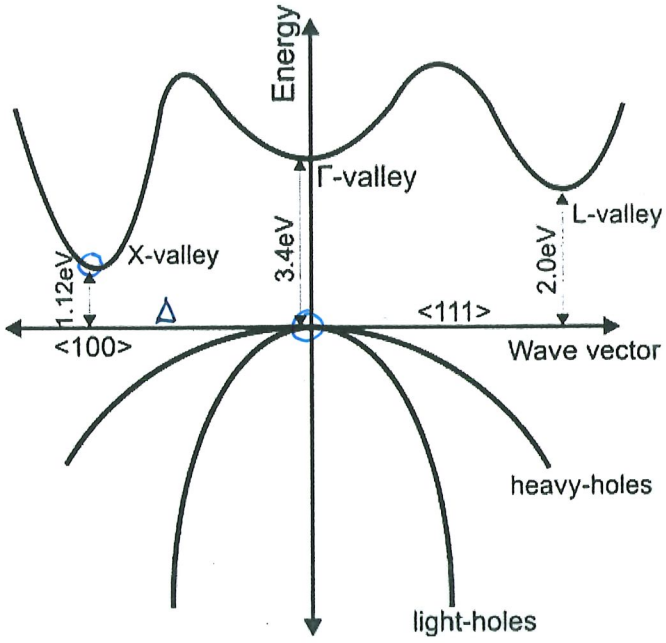
Silicon

- Minimum of CB (lowest) is at ~80% from Γ to X
  near X
- Top of VB is at Γ
  ∴ Indirect Gap (~1.1 eV)

There are 6 CB minima because there are 6 paths from $\vec{k}=0$ (Γ-point) to X (along $\pm k_x, \pm k_y, \pm k_z$).



Simplified Picture



Pockets ("X-valleys") of electrons in CB

- When there are electrons (thermal excitation or doping) filling states in CB, they start with the lowest states near the 6 minima

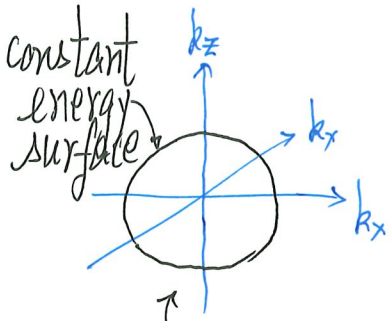
  ⇒ **6 pockets of electrons near the 6 minima**

Constant Energy Surface(s)

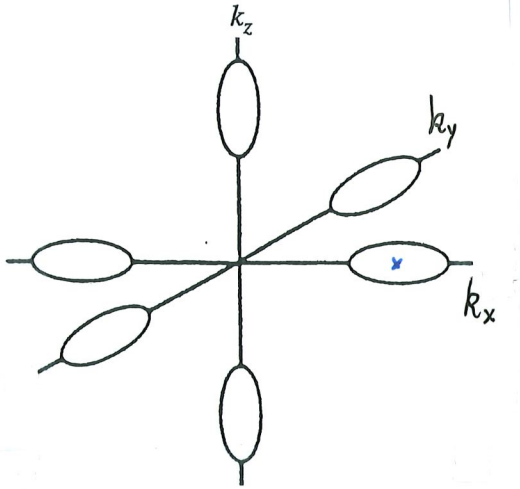
Free particle example

$$\mathcal{E}(\vec{k}) = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

For given number of electrons (electron density), they fill the states from minimum ($\vec{k}=0$) up. After all electrons are filled in, the last ones filled states on a spherical constant energy surface.



volume enclosed (area of surface) depends on number of electrons

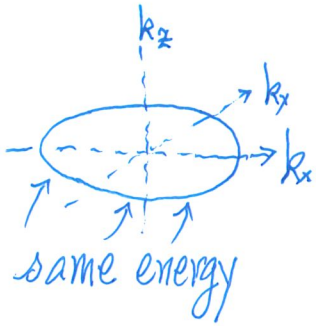


Six constant-energy surfaces for electrons in Silicon

6 ellipsoids (band is anisotropic near CB minima)

Volume enclosed (area of ellipsoids) depends on number of electrons (electron number density)

- Consider minimum at $(+k_0, 0, 0) \equiv \vec{k}_0$

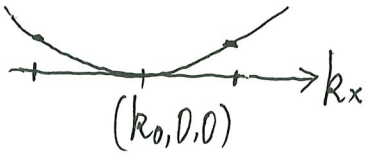


Around the minimum (a point (k_x, k_y, k_z) near $(k_0, 0, 0)$)

$$E_{CB}(\vec{k}) = E_{CB}(\vec{k}_0) + \frac{\hbar^2(k_x - k_0)^2}{2m_l^*} + \frac{\hbar^2 k_y^2 + \hbar^2 k_z^2}{2m_t^*} \quad (2)$$

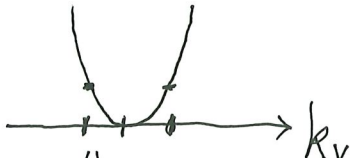
↑ two different effective masses

same energy: $(k_x - k_0)$ goes farther than k_y (k_z)



m_l^*

$(m_l^* > m_t^*)$

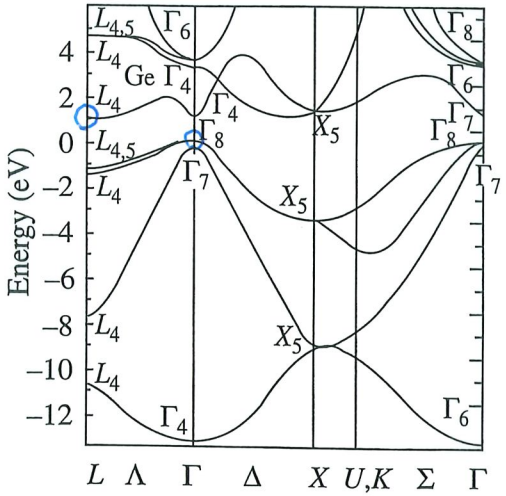


m_t^*

$m_l^* = 0.98\, m_e$

$m_t^* = 0.19\, m_e$

Germanium



Band structure of Ge (after Chelikowsky and Cohen 1976).

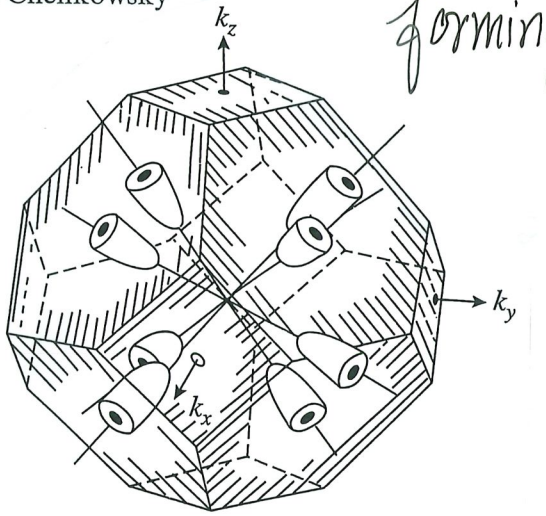
Bottom of CB is at L (from Γ in ⟨111⟩ directions to Zone edge)

Top of VB's at $\vec{k}=0$

Indirect Gap ~ 0.74 eV

There are 8 CB minima

When electrons fill into states near the CB minima, there are 8 half-ellipsoids (add up to 4 ellipsoids) forming the pockets of filled CB electronic states



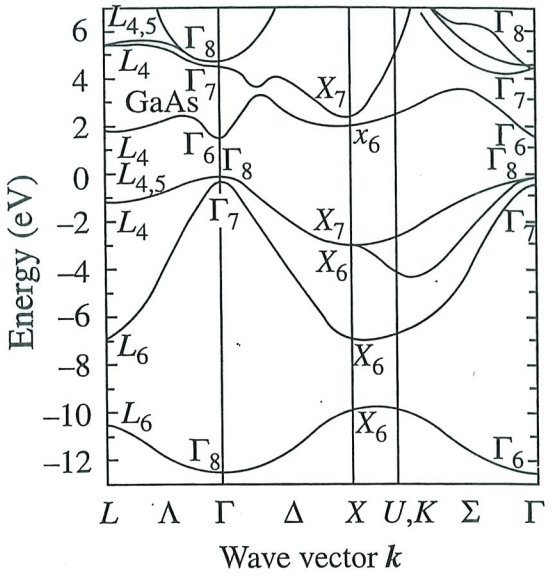
Constant energy surfaces for the conduction band of Ge.

$m_\ell^* = 1.64\, m_e$

$m_t^* = 0.082\, m_e$

after rotating ellipsoids to 

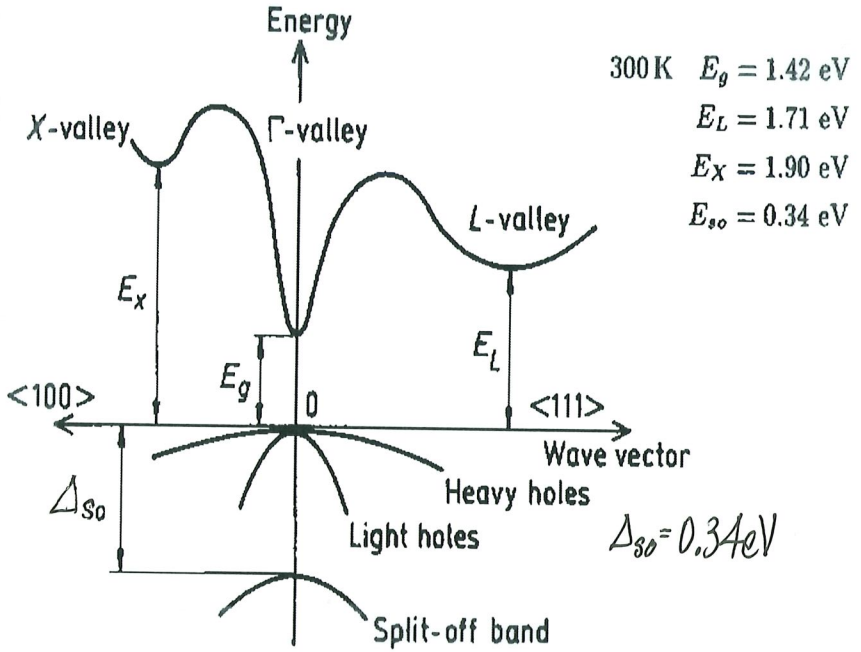
GaAs



Band structure of GaAs (after Chelikowsky and Cohen 1976).

Bottom of CB at Γ and Top of VB's at Γ

Direct Gap ~ 1.424 eV



CB $m^* = 0.067\, m_e$

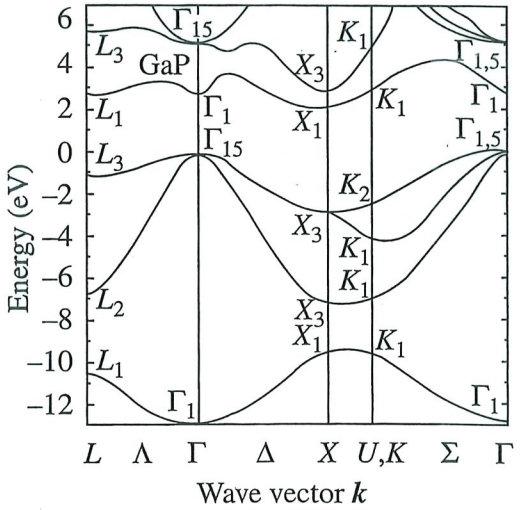
↑ ~6.7% of m_e

(isotropic)

Schematic GaAs Band Structure to keep in mind

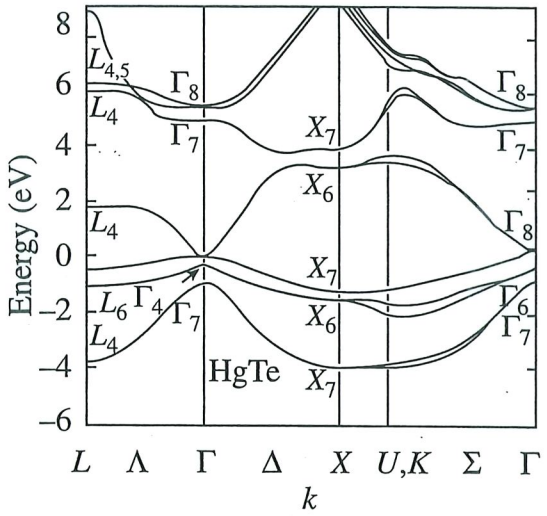
Other materials

GaP



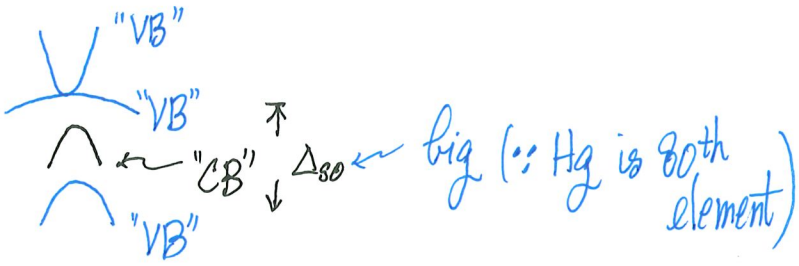
Band structure of GaP (after Chelikowsky and Cohen 1976).

HgTe



Band structure of HgTe (after Cohen and Chelikowski 1988).

Not a semiconductor
[zero gap (or negative gap) with overlapping VB and CB]
(a semimetal)



← big (∵ Hg is 80th element)

HgTe is important because when it is alloyed with Cd ($Cd_xHg_{1-x}Te$), a gap can be opened with E_g depending on x.

C. Electron Effective Mass

Motivation:

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2) \quad \text{(isotropic)}$$

$$\frac{1}{m_e} = \frac{1}{\hbar^2}\frac{\partial^2 E(k)}{\partial k^2}$$

[m_e = bare electron mass]

Real band structures are in general anisotropic and there are many bands

$$\left(\frac{1}{m^*}\right)_{\alpha\beta} = \frac{1}{\hbar^2}\frac{\partial^2 E(\vec{k})}{\partial k_\alpha \partial k_\beta} \qquad (3)$$

an inverse effective mass tensor (matrix)

$\alpha, \beta = x, y, z$

c.f. Free particle

$$\frac{1}{\hbar^2}\frac{\partial^2 E(\vec{k})}{\partial k_\alpha \partial k_\beta} = \frac{1}{m}\delta_{\alpha\beta}$$