Lecture contents

- Free and crystal electrons
- Holes
- Few experimental techniques for bandstructure determination
  - UPS
  - ECR

Free electrons and crystal electrons

Free electrons

Wave function: $$\psi_k(r) = \frac{1}{\sqrt{V}} e^{ikr}$$

Kinetic energy: $$E = \frac{\hbar^2 k^2}{2m}$$

Velocity or group velocity:

$$\bar{v} = \int \psi^* \left(-\frac{i\hbar}{m} \nabla \right) \psi dr = \frac{\hbar k}{m}$$

Dynamics (F – force):

$$\frac{dv}{dt} = \frac{1}{m} F$$

Force equation:

$$F = \frac{dp}{dt} = \hbar \frac{dk}{dt}$$

Electrons in semiconductor

Wave function: $$\psi_k(r) = e^{ikr} u_k(r)$$

Dispersion near band extremum (isotropic and parabolic): $$E = \frac{\hbar^2 (k - k_0)^2}{2m^*}$$

Group velocity: $$v = \frac{1}{\hbar} \nabla_k E(k)$$

Velocity at band extremum: $$v = \frac{\hbar (k - k_0)}{m^*}$$

Dynamics at band extremum:

$$\frac{dv}{dt} = \frac{1}{\hbar} \nabla_k \frac{dE}{dt} = \frac{1}{\hbar} \nabla_k (Fv) = \frac{1}{\hbar^2} (\nabla_k \nabla_k E) F$$

$$\frac{dv}{dt} = \frac{1}{m^*} F; \qquad \frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}$$ (if m* isotropic and parabolic)

Force equation:

$$\frac{dE(k)}{dt} = \nabla_k E \frac{dk}{dt} = Fv$$

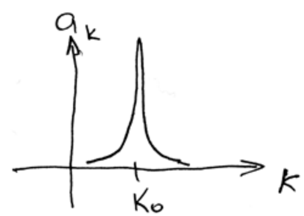
$$F = \hbar \frac{dk}{dt}$$

Group velocity

Wave packet at $k = k_0$

$$f_{k_0}(r,t) = \int a_k \, \psi_k(r,t) \, d^3k$$

$$\psi_k(r,t) = e^{ikr} u_k(r) e^{-i\frac{E_k}{\hbar}t}$$



$$E_k = E_{k_0} + \Delta k \cdot \nabla_k E_{k_0} + \dots$$

$$u_k = u_{k_0} + \Delta k \, \nabla_k u_{k_0} + \dots$$

$$a_k \equiv a_{\Delta k}$$

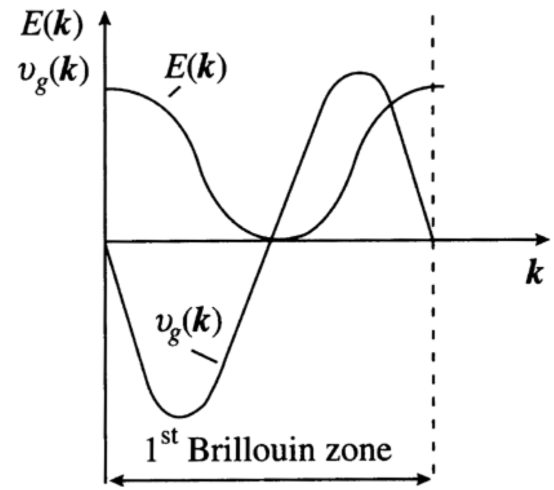
$$f_{k_0}(r,t) = e^{ik_0 r} u_{k_0} e^{-i\frac{E_{k_0}}{\hbar}t} \int a_{\Delta k} \, e^{i\Delta k\left[r - \nabla_k E_{k_0}\frac{t}{\hbar}\right]} d^3k + \dots \text{small}$$

at $\quad r - \frac{t}{\hbar}\nabla_k E_{k_0} = \text{const}$

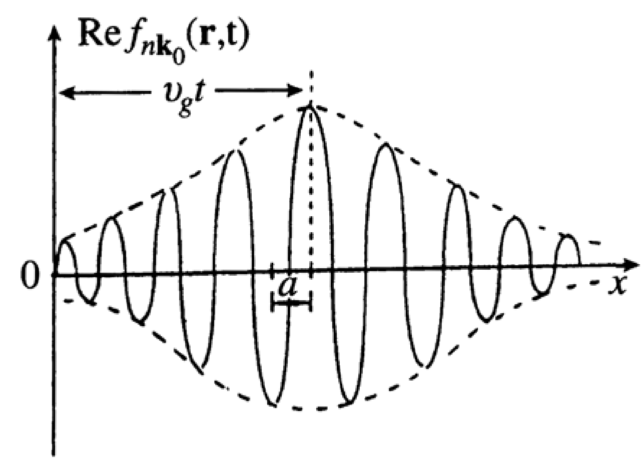
$$v_g = \frac{r}{t} = \frac{1}{\hbar}\nabla_k E_{k_0}$$

$$\Delta r \approx \frac{1}{\Delta k} >> a_0$$

Dispersion and group velocity:



Wave packet in real space:

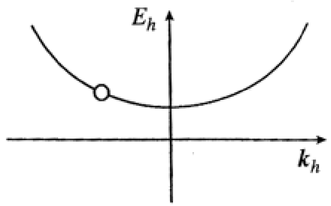


Group velocity applet
[http://galileo.phys.virginia.edu/classes/109N/more_stuff/Applets/sines/GroupVelocity.html]

Holes

- It is convenient to treat top of the uppermost valence band as hole states

Hole energy:



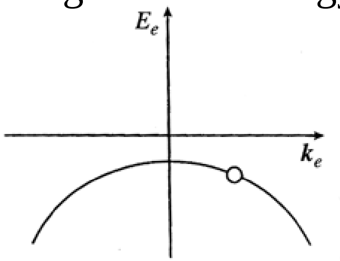
- Wavevector of a hole = total wavevector of the valence band (=zero) minus wavevector of removed electron:

$$k_h = 0 - k_e$$

- Energy of a hole. Energy of the system increases as missing electron wavevector increases:

$$E_h(k_h) = -E_e(k_e)$$

Missing electron energy:



$$E_e(k_e) = E_v + \frac{\hbar^2 k_e^2}{2m_e^*}$$

- Mass of a hole. Positive! (Electron effective mass is negative!)

$$m_h^* = -m_e^* \qquad E_h(k_h) = -E_v + \frac{\hbar^2 k_h^2}{2m_h^*}$$

- Group velocity of a hole is the same as of the missing electron

$$v_h = \frac{1}{\hbar}\nabla_k E_h(k_h) = \frac{1}{\hbar}\nabla_k\left[-E_e(-k_e)\right] = v_e$$

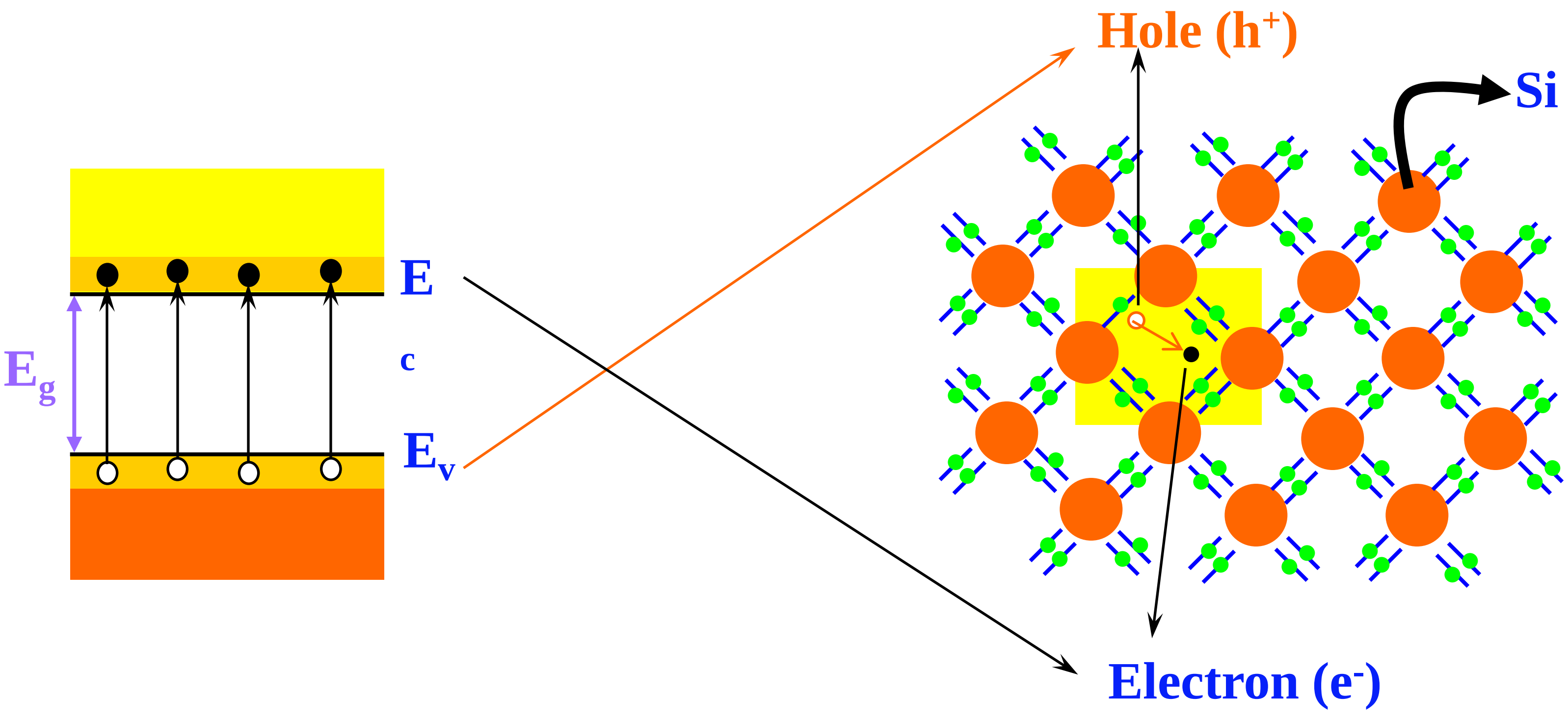
- Charge of a hole. Positive!

$$\hbar\frac{dk_e}{dt} = -e\mathcal{E}$$

$$\hbar\frac{dk_h}{dt} = e_h\mathcal{E}$$

$$e_h = -e_e = +e$$

Example: electron-hole pairs



EHP generation : Minimum energy required to break covalent bonding is E_g.

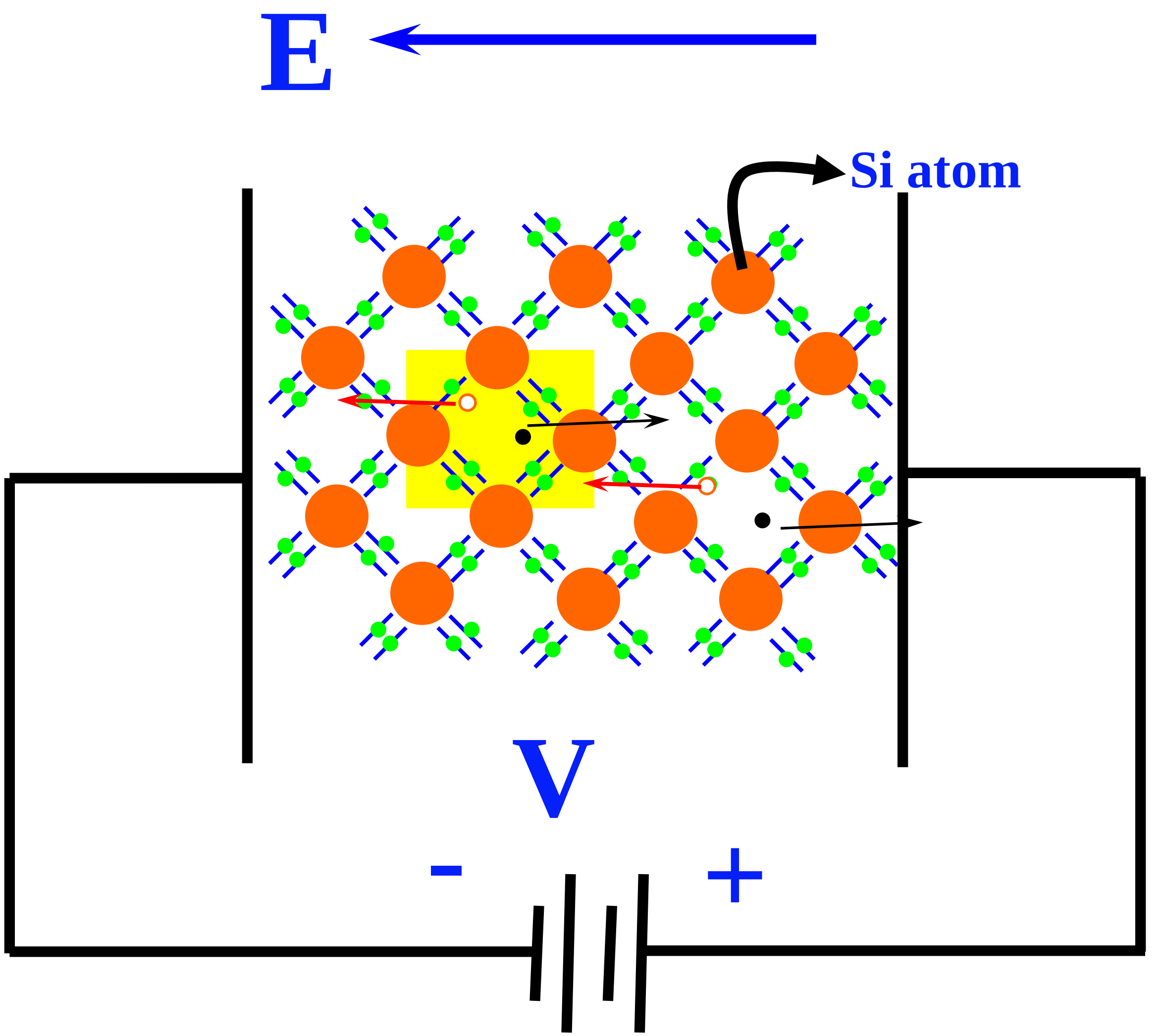
Charge carriers in a crystal

$$F = ma = +qE$$

hole

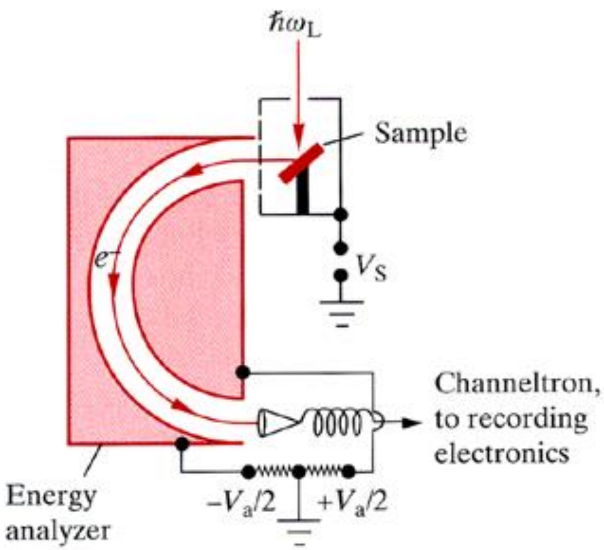
$$F = ma = -qE$$

electron



Charge carriers in a crystal are not completely free. ➔ Need to use effective mass NOT REST MASS !!!

Angle-resolved photoelectron spectroscopy (UPS): Band structure determination



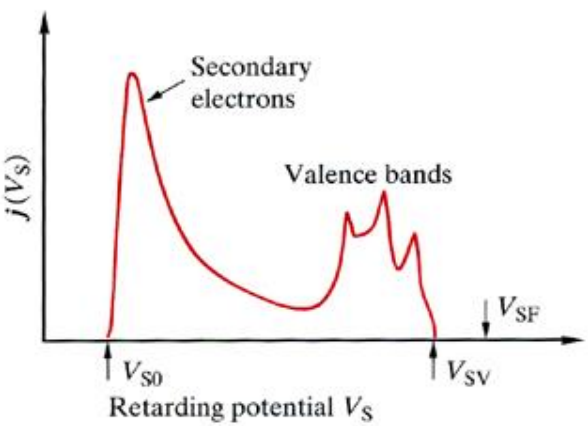


Fig. 8.12. Schematic diagram of a typical angle-integrated photoelectron spectrum

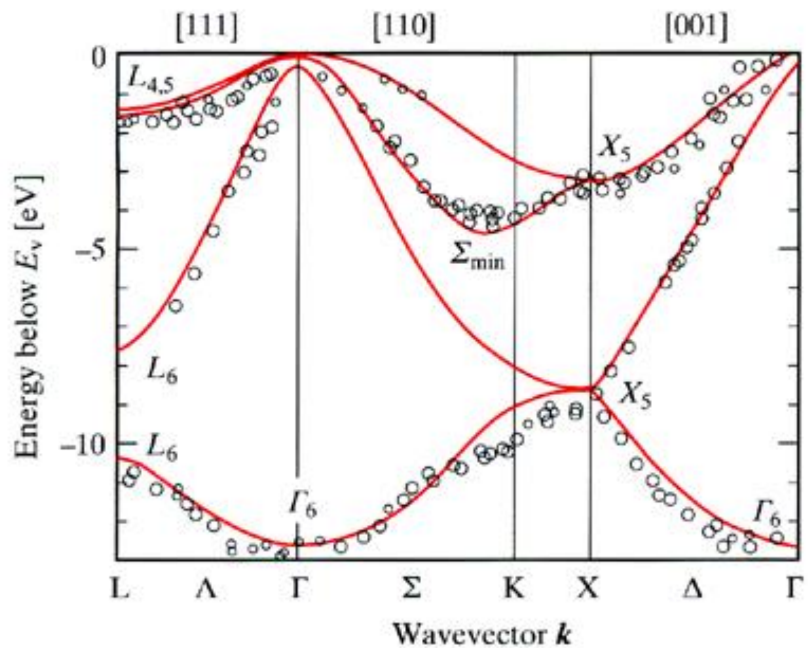


Fig. 8.19. Valence band structure of Ge determined by angle-resolved UPS, compared with the results of a theoretical prediction (*solid lines*) [8.41].

Photo-threshold energy (from E_V to vacuum)

$$I = \hbar\omega_L - e(V_{SV} - V_{SO})$$

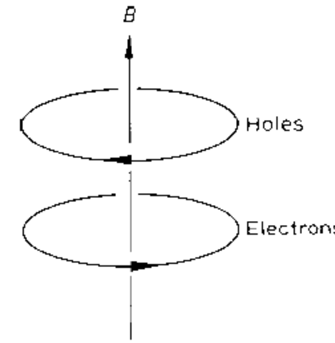
From Yu and Cordona, 2003

Cyclotron resonance: effective mass determination

Lorentz force on a moving particle $$F_m = e(v \times B)$$

Centripetal force for circular motion $$F_c = m\frac{v^2}{r}$$

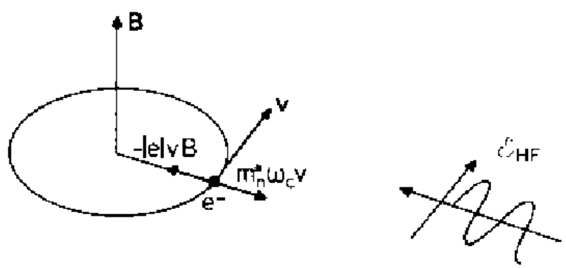
Cyclotron frequency (does not depend on *v* !) $$\omega_c = \frac{v}{r} = \frac{|e|B}{m^*}$$



Set-up:

- Place crystal in static magnetic field ***B***
- measure absorption of RF electric field ***E***
- keep ***E*** constant and change ***B:*** $\mu(B)$

Very pure crystals
Low Temperature
Illuminate sample



Large mean free path of carriers (long scattering times) $$\tau\omega_c > 1$$

Cyclotron resonance: effective mass determination

In real semiconductors effective mass m_{e*} may depend on the direction. These different effective masses can be measured by varying the angle of ***B*** with respect to the crystallographic axes.

- In real space: Electrons move on closed orbits.
- In *k*-space: Electrons and holes move along constant energy surfaces in planes perpendicular to ***B***.
- In crystals both orbits (*k*-space, real space) are no longer circular: When the effective mass is anisotropic, the orbits become ellipsoidal.
- For electrons in Si:

Si

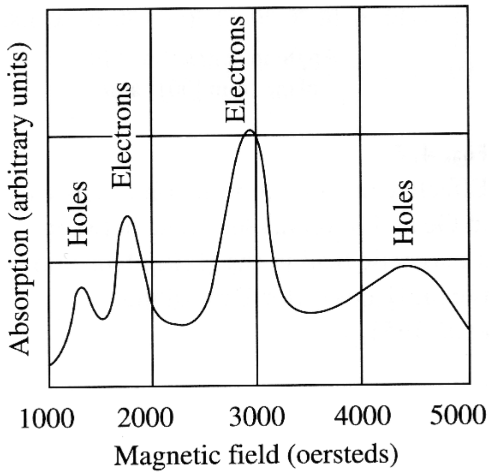
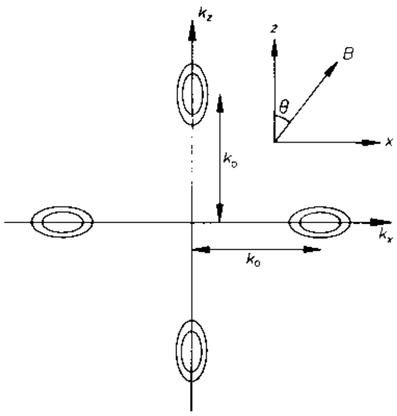


Fig. 4.6
Cyclotron resonance absorption versus magnetic field at 24000 Mc/s for Si at 4 K (after Dresselhaus *et al.* 1955).

$$E = \frac{\hbar^2}{2}\left(\frac{k_x^2 + k_y^2}{m_T} + \frac{(k_z - k_0)^2}{m_L}\right)$$

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{v} \times \vec{B}$$

$$\vec{v} = \frac{1}{\hbar}\vec{\nabla}_k E$$



Cyclotron resonance in Ge

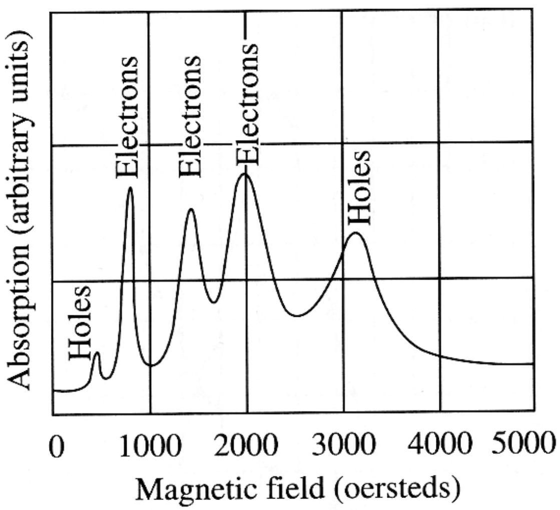


Fig. 4.5
Cyclotron resonance absorption versus magnetic field at 24000 Mc/s for Ge at 4 K (after Dresselhaus *et al.* 1955).

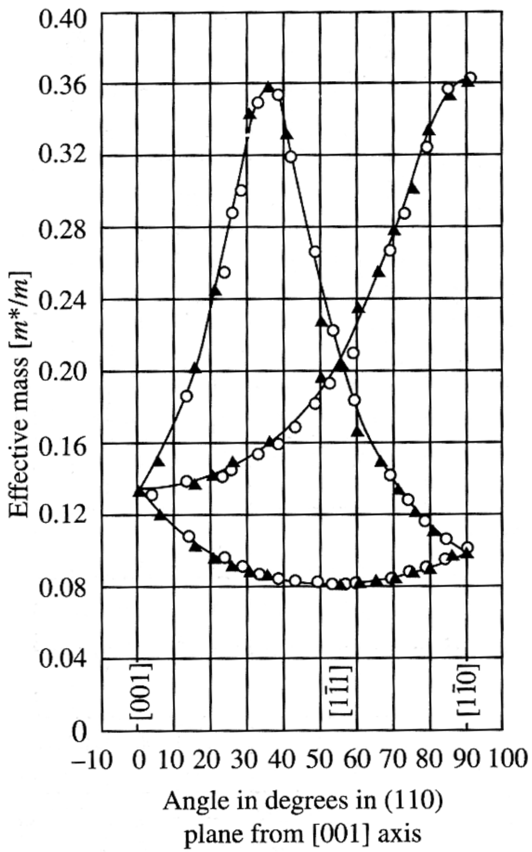
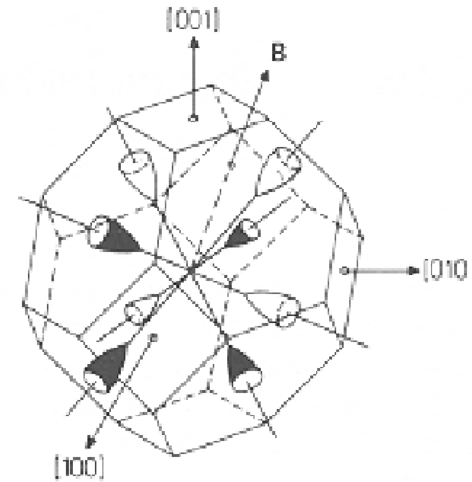
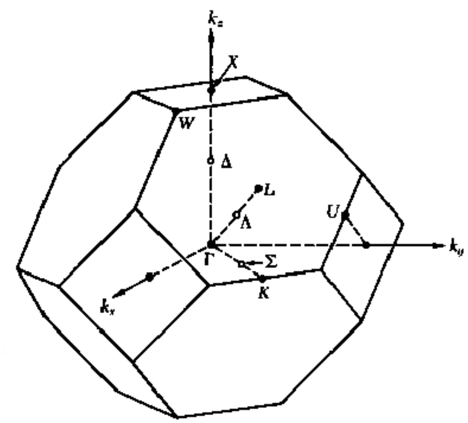


Fig. 4.7
Effective mass of conduction electrons in Ge at 4 K versus the angle between a magnetic field in the (110) plane and the [001] axis (after Dresselhaus *et al.* 1955).





From Balkanski and Wallis, 2000