

# Lecture contents

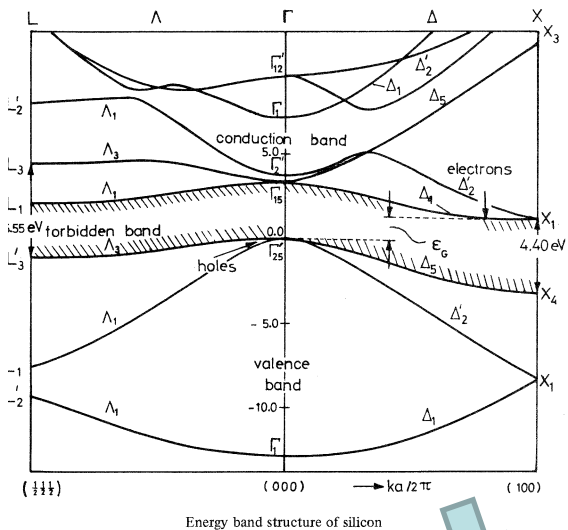
- Semiconductor bands
- Effective mass
- Holes in semiconductors
- Semiconductor alloys

|   |   |  |  |   |
|---|---|--|--|---|
| Group<br>2a                                       |   |  |  |   |
| <sup>4</sup><br><b>Be</b><br>Beryllium<br>9.0122  | Group<br>3a                                       | Group<br>4a                                      | Group<br>5a  | Group<br>6a                                       |
| <sup>12</sup><br><b>Mg</b><br>Magnesium<br>24.305 | <sup>5</sup><br><b>B</b><br>Boron<br>10.811       | <sup>6</sup><br><b>C</b><br>Carbon<br>12.011     | <sup>7</sup><br><b>N</b><br>Nitrogen<br>14.0067    | <sup>8</sup><br><b>O</b><br>Oxygen<br>15.9994     |
| Group<br>2b                                       | <sup>13</sup><br><b>Al</b><br>Aluminum<br>26.9815 | <sup>14</sup><br><b>Si</b><br>Silicon<br>28.086  | <sup>15</sup><br><b>P</b><br>Phosphorus<br>30.9738 | <sup>16</sup><br><b>S</b><br>Sulfur<br>32.066     |
| <sup>30</sup><br><b>Zn</b><br>Zinc<br>65.39       | <sup>31</sup><br><b>Ga</b><br>Gallium<br>69.72    | <sup>32</sup><br><b>Ge</b><br>Germanium<br>72.61 | <sup>33</sup><br><b>As</b><br>Arsenic<br>74.9216   | <sup>34</sup><br><b>Se</b><br>Selenium<br>78.96   |
| <sup>48</sup><br><b>Cd</b><br>Cadmium<br>112.41   | <sup>49</sup><br><b>In</b><br>Indium<br>114.82    | <sup>50</sup><br><b>Sn</b><br>Tin<br>118.71      | <sup>51</sup><br><b>Sb</b><br>Antimony<br>121.76   | <sup>52</sup><br><b>Te</b><br>Tellurium<br>127.60 |
| <sup>80</sup><br><b>Hg</b><br>Mercury<br>200.59   | <sup>81</sup><br><b>Tl</b><br>Thallium<br>204.38  | <sup>82</sup><br><b>Pb</b><br>Lead<br>207.2      | <sup>83</sup><br><b>Bi</b><br>Bismuth<br>208.98    | <sup>84</sup><br><b>Po</b><br>Polonium<br>(210)   |

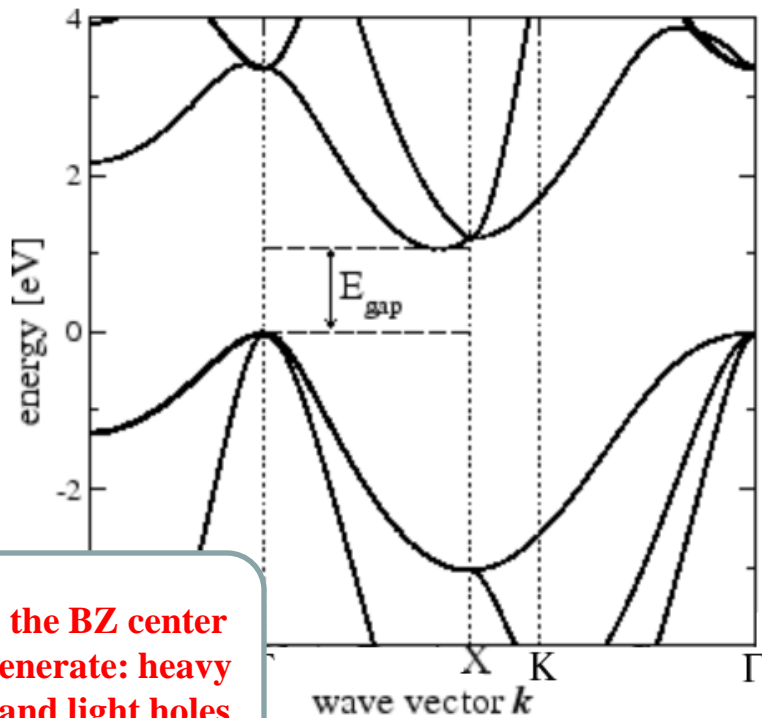
# Band-structure of Si

Conduction band valleys in Si

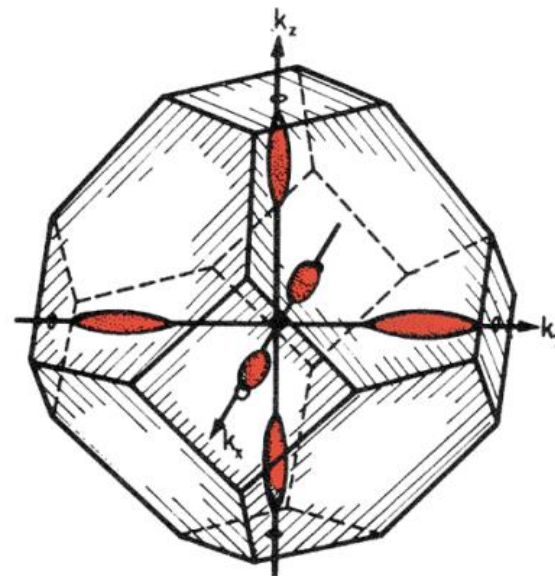
$$\mathbf{k}_{\min} = \frac{2\pi}{a_0}(0, 0, 0.85) = (0, 0, k_{\min})$$



Energy band structure of silicon



**VB in the BZ center is degenerate: heavy holes and light holes**

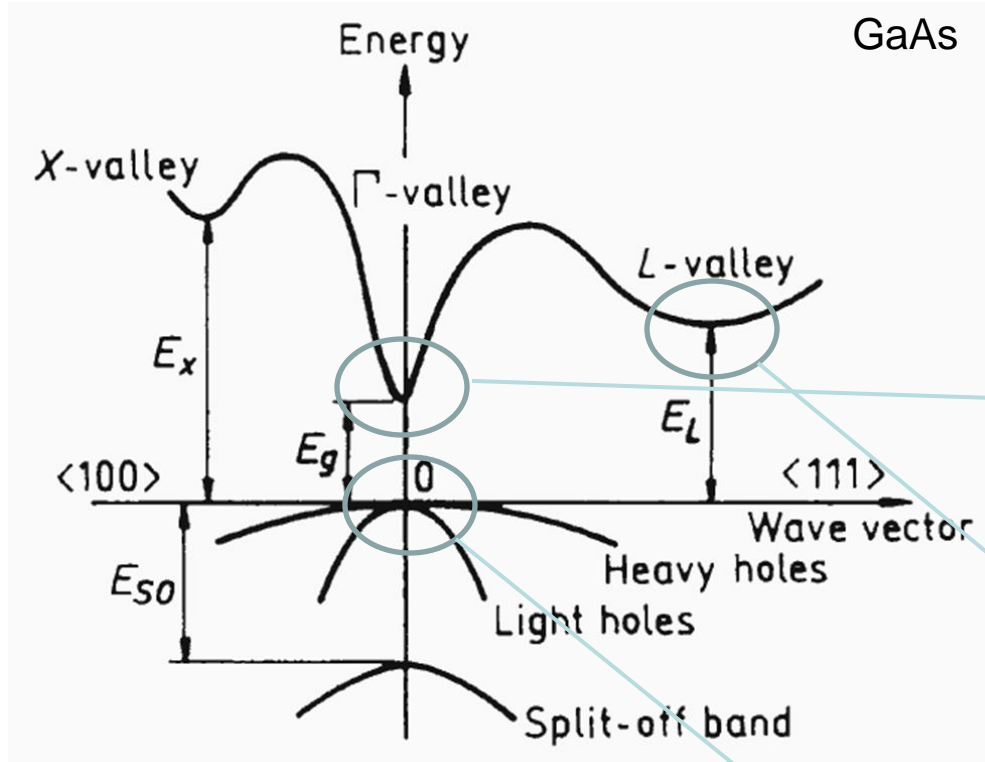


$$E(\mathbf{k}) = \frac{\hbar^2 (k_z - k_{\min})^2}{2m_l} + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_t}$$

|    | $m_l^*$ | $m_t^*$ | $\bar{m}_{lh}^*$ | $\bar{m}_{hh}^*$ |
|----|---------|---------|------------------|------------------|
| Si | 0.92    | 0.19    | 0.16             | 0.52             |
| Ge | 1.59    | 0.082   | 0.043            | 0.34             |

# Density of states in 3D and DOS effective mass

## Effective mass density of states



3D density of states

$$N(E) = \frac{\sqrt{2}m^{*3/2}}{\pi^2\hbar^3} (E - V_0)^{1/2}$$

Conduction band DOS mass in  $\Gamma$  point:

$$m_{dos}^* = m_c^*$$

Conduction band DOS mass in indirect gap semiconductors ( $\xi_c$ - degeneracy of the valley):

$$m_{dos}^* = \xi_c^{2/3} (m_1^* m_2^* m_3^*)^{1/3}$$

Valence band DOS mass :

$$m_{dos}^* = \left( m_{hh}^{*3/2} + m_{lh}^{*3/2} \right)^{2/3}$$

# Free electrons and crystal electrons

Free electrons

Electrons in solid

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

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

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

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

Velocity or group velocity:

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

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

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

Dynamics ( $F$  – force):

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

Dynamics in a band:

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

Force equation:

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

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

Force equation:

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

# Holes

- It is convenient to treat top of the uppermost valence band as hole states
- Wavevector of a hole = total wavevector of the valence band (=zero) minus wavevector of removed electron:
- Energy of a hole. Energy of the system increases as missing electron wavevector increases:
- Mass of a hole. Positive! (Electron effective mass is negative!)

$$m_h^* = -m_e^*$$

$$k_h = 0 - k_e$$

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

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

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

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

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

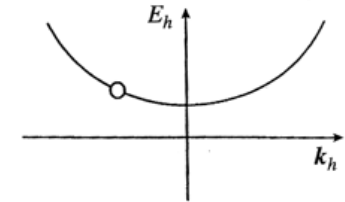
- Charge of a hole. Positive!

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

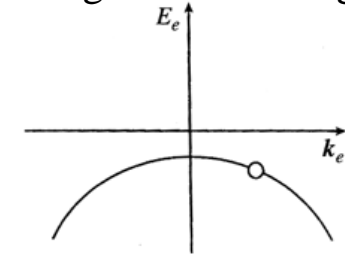
$$\hbar \frac{dk_h}{dt} = e_h \mathcal{E}$$

$$e_h = -e_e = +e$$

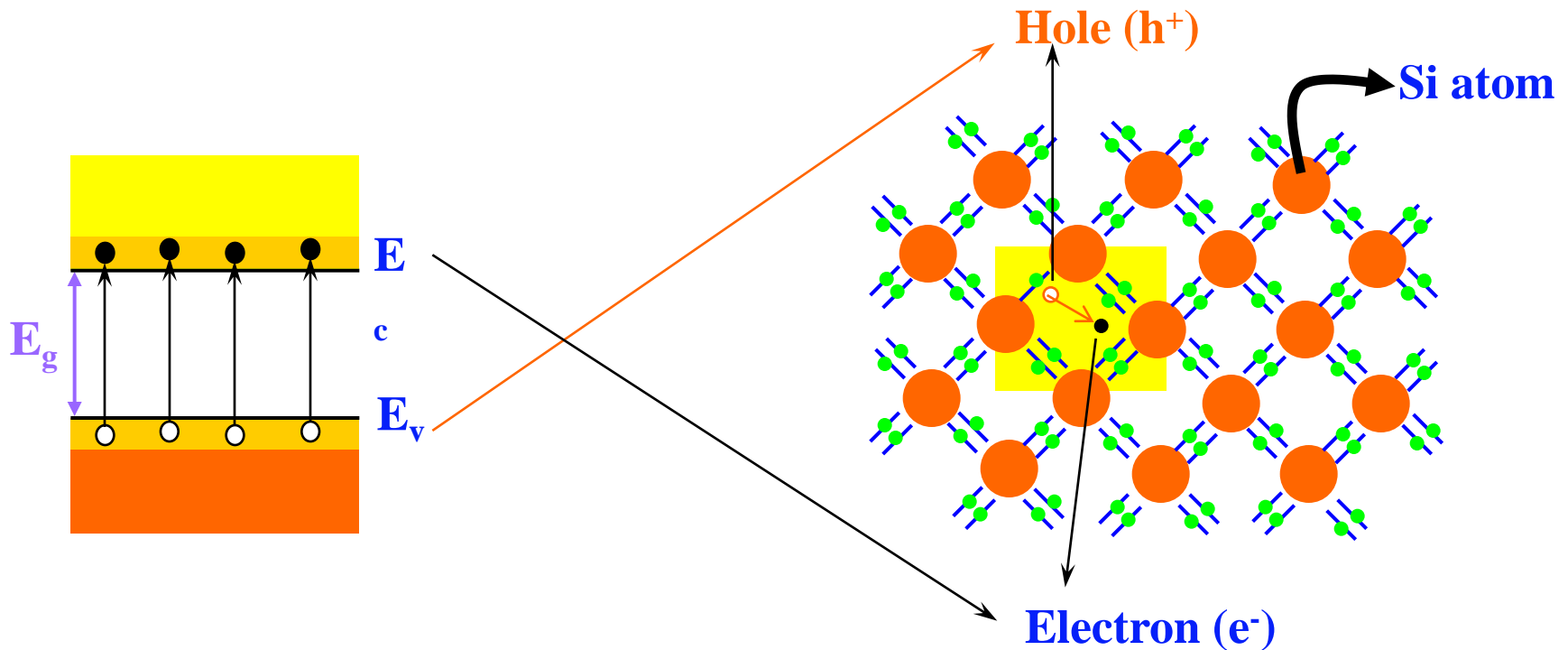
Hole energy:



Missing electron energy:



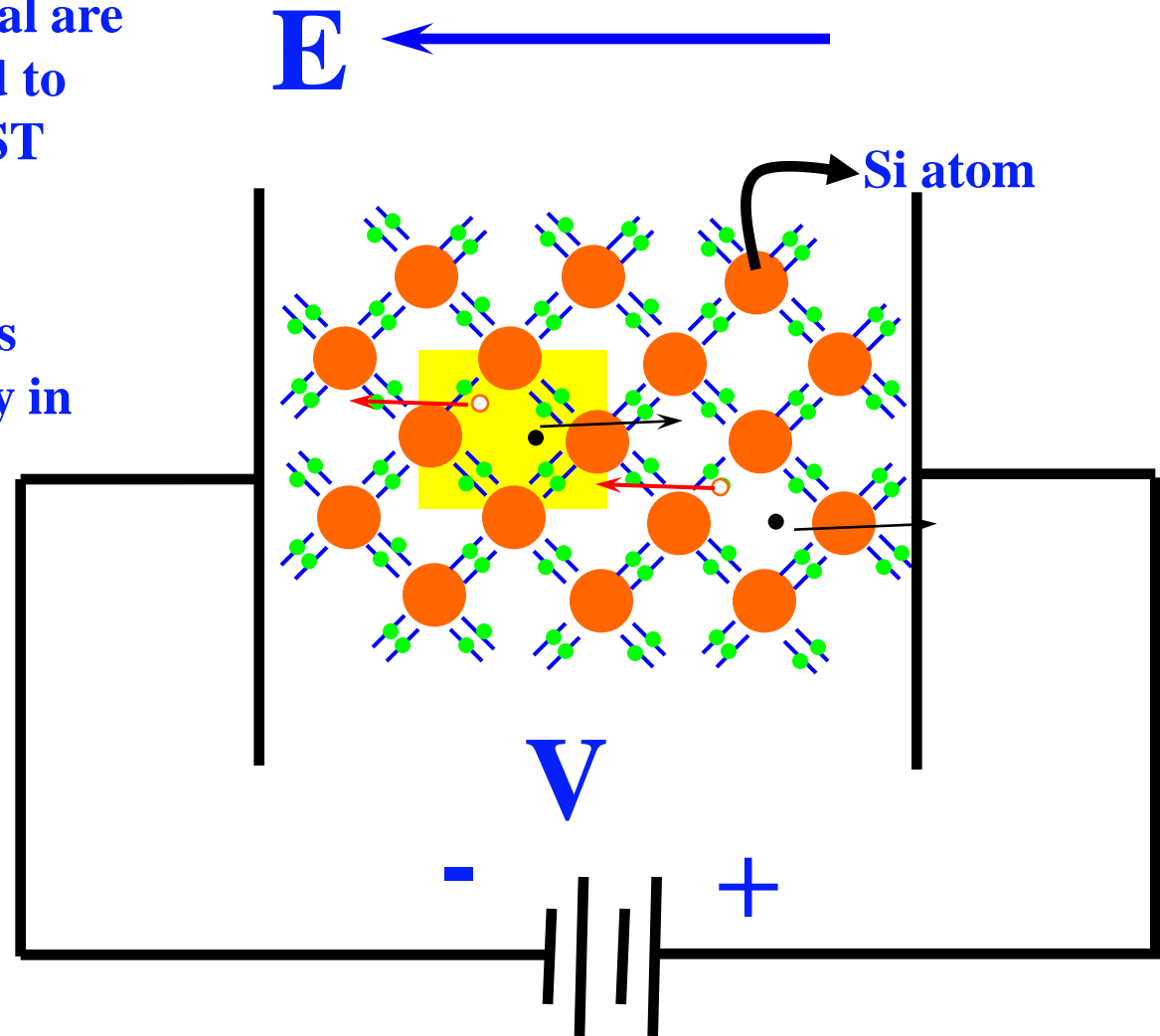
# Example: electron-hole pairs in semiconductors



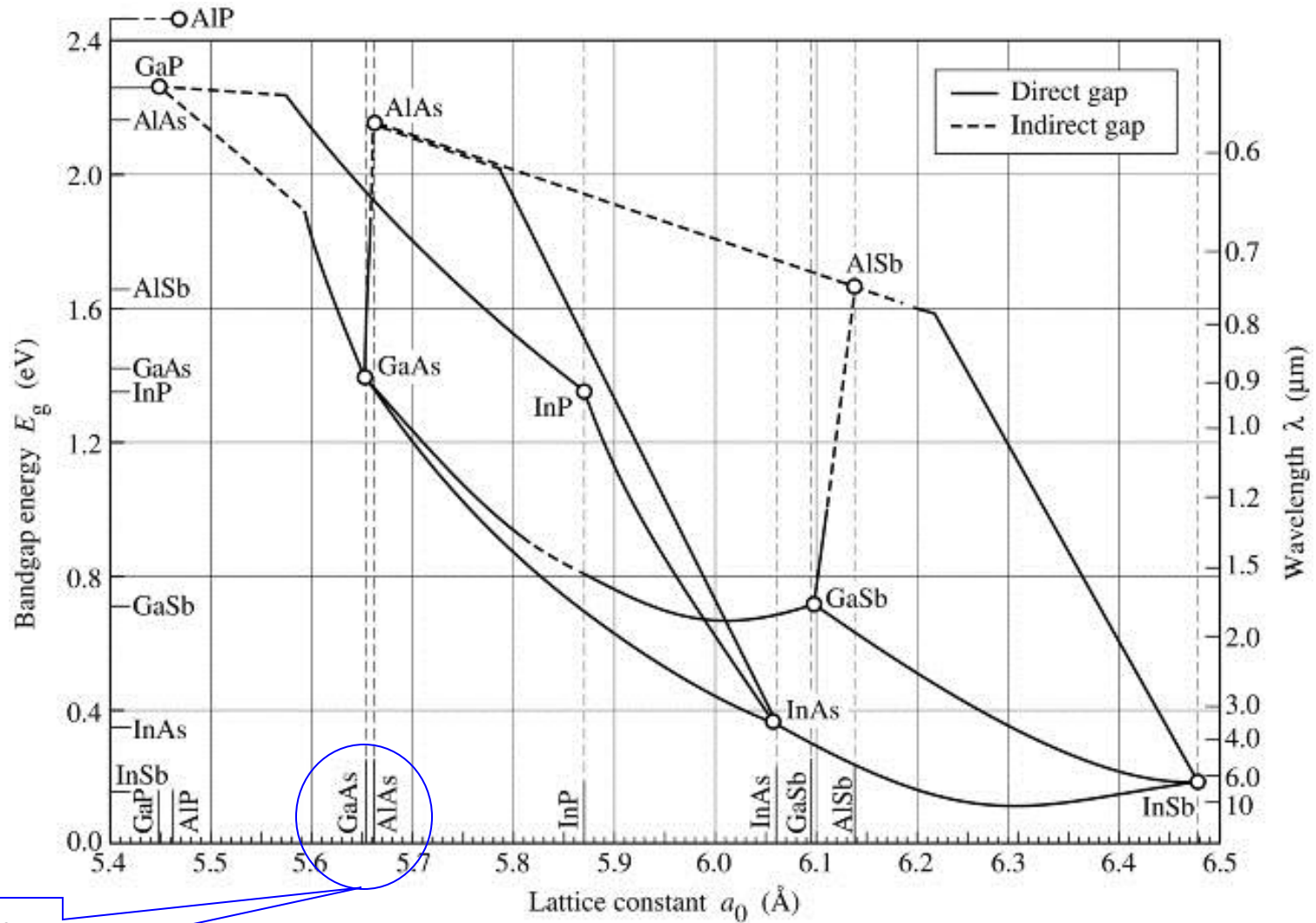
**EHP generation : Minimum energy required to break covalent bonding is  $E_g$ .**

## Charge carriers in a crystal

- Charge carriers in a crystal are not completely free. → Need to use effective mass NOT REST MASS !!!
- Electron and hole currents have to be treated separately in devices



# Bandgap and lattice constants



Very close  
lattice  
matching

Fig. 7.6. Bandgap energy and lattice constant of various III-V semiconductors at room temperature (adopted from Tien, 1988).



# Alloys

Vegard's law for lattice constant of alloy

Works for

- Random alloys
- With constant crystal structure

Average periodic potential of a “virtual crystal”

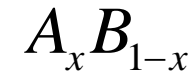
$$V_{\text{alloy}} = xV_A + (1-x)V_B$$

Band extrema follow almost linear dependence with slight bowing due to alloy disorder

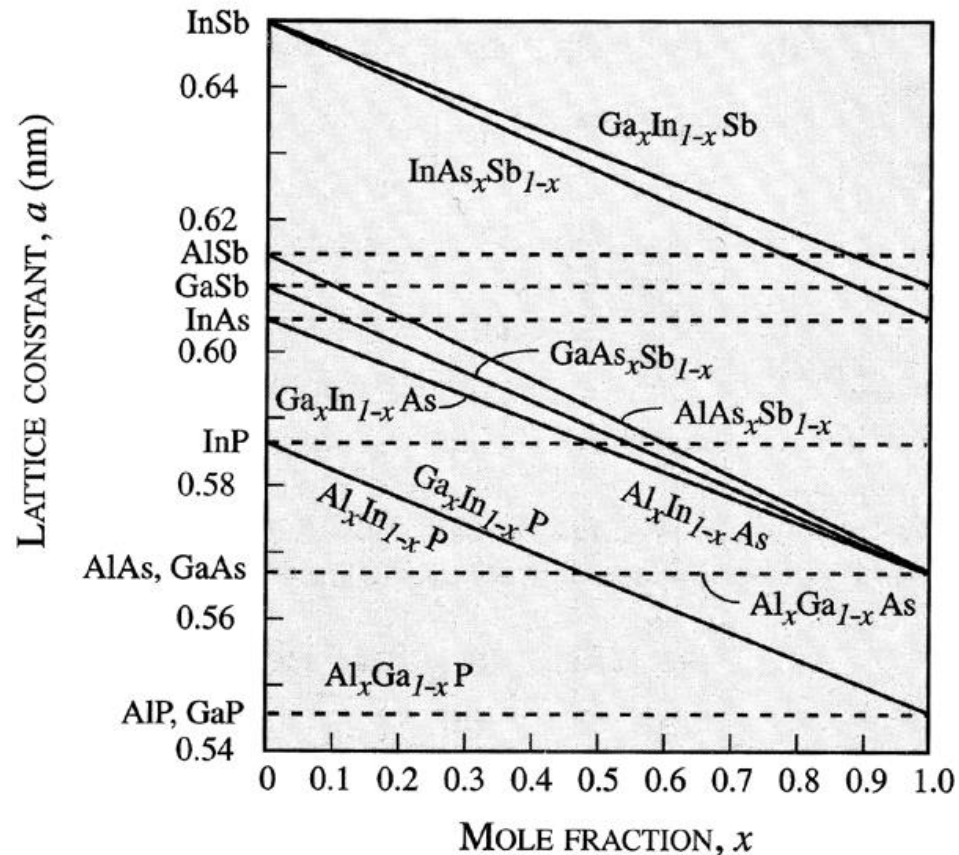
$$E_g^{\text{alloy}} = a + bx + cx^2$$

Effective mass for a given extremum

$$\frac{1}{m_{\text{alloy}}^*} = \frac{x}{m_A^*} + \frac{1-x}{m_B^*}$$



$$a_{\text{alloy}} = xa_A + (1-x)a_B$$



From Singh, 2003

# Bandgap in AlGaAs

## Bandgap of AlGaAs

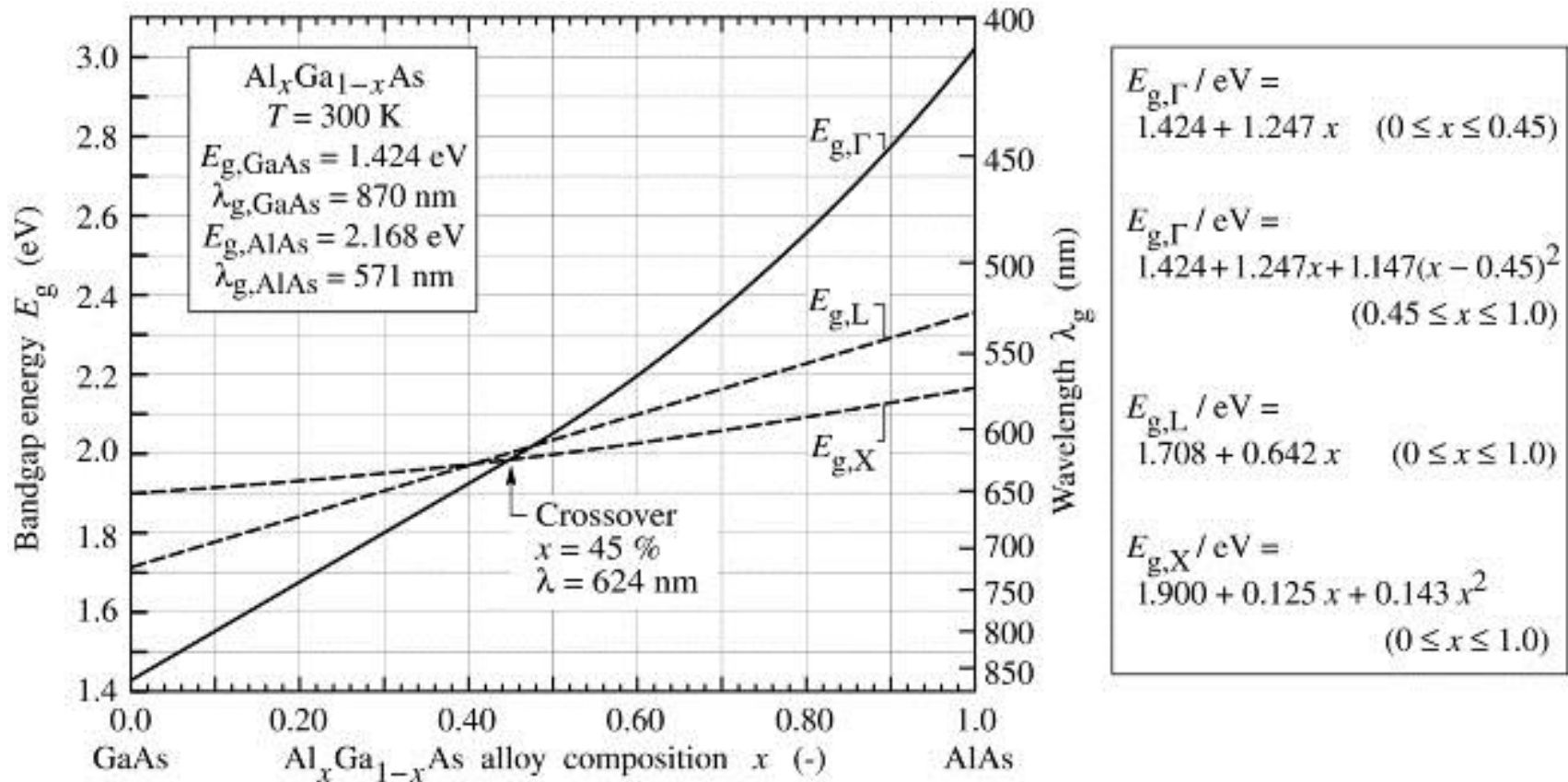
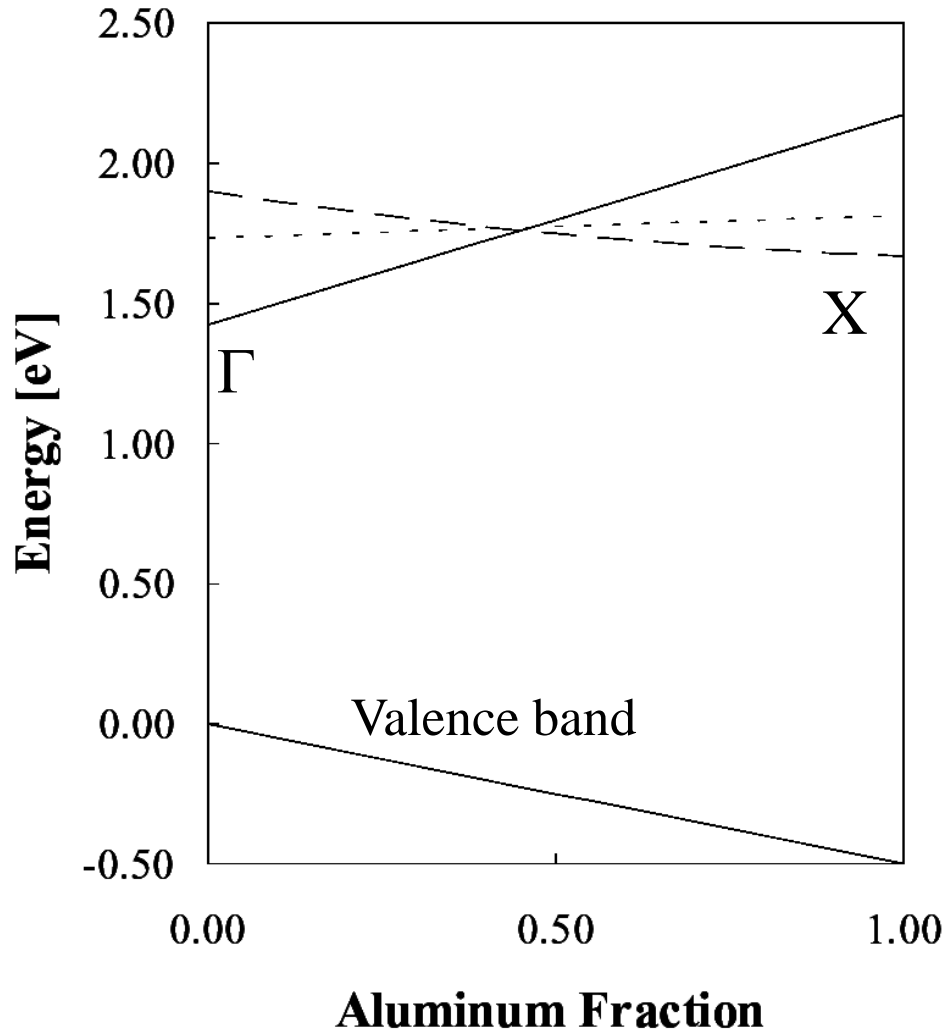


Fig. 7.7. Bandgap energy and emission wavelength of AlGaAs at room temperature.  $E_{\Gamma}$  denotes the direct gap at the  $\Gamma$  point and  $E_L$  and  $E_X$  denote the indirect gap at the L and X point of the Brillouin zone, respectively (adopted from Casey and Panish, 1978).

# Bandgap in AlGaAs

Bandgap of AlGaAs related to the vacuum level



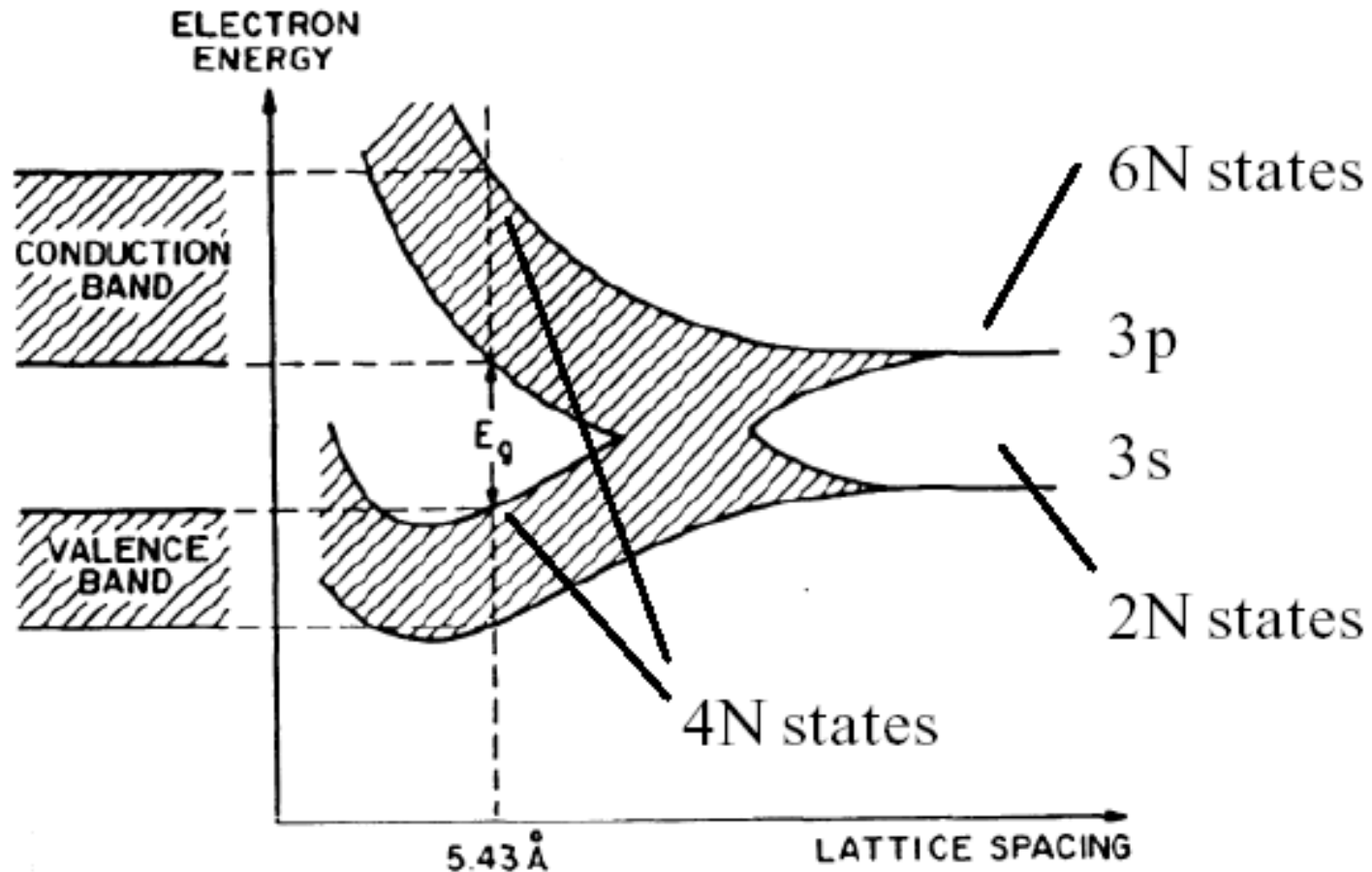
- Knowledge of band edge positions is important in junctions

## Temperature dependence of the energy bandgap

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

|                      |                        | Germanium | Silicon | GaAs  |
|----------------------|------------------------|-----------|---------|-------|
| Bandgap at T = 0K    | $E_g(0)$ [eV]          | 0.7437    | 1.166   | 1.519 |
| Coefficient $\alpha$ | $[10^{-4} / \text{K}]$ | 4.774     | 4.73    | 5.405 |
| Coefficient $\beta$  | [K]                    | 235       | 636     | 204   |

## Energy bands in semiconductors



- Bandgap dependence on temperature is mostly due to thermal expansion

## Lecture recap

- In semiconductors extrema of CB and VB are most important
- VB in the BZ center is degenerate: heavy holes and light holes
- Holes as “independent” quasi-particles
- Vegards’ law
- Bandgap dependence on temperature