

# Band structure of solid state

Considering the knowledge of molecules each atomic energy level will split into two sublevels (bonding and anti-bonding state) if two atoms are approaching to a distance  $d$ . In solid there are several of such next neighbour distances resulting in a lot of overlapping states- energy bands. These energy band describe allowed states for electrons separated by energy gaps where now allowed state exist. In a very simple 1D model each electron band can be described by

$$E(k, m) = E_m^{at} - \alpha_m - 2\beta_m \cos(ka)$$

Where  $\alpha_m$  describes the reduction of atomic energy due to chemical bond and  $4\beta_m$  the width of the energy band..  $k = \frac{2\pi}{\lambda}$  is the electron momentum. The lower band level is at  $k=0$  and the upper level at  $k = \frac{\pi}{a}$ .

An alternative approach is a description of band structure in reciprocal space, considering the electron momentum  $p = \hbar k$ , subsequently the electron energy can be described by

$$E(k) = \frac{\hbar^2}{2m} k^2$$

In this approach the electron can be assumed to form standing waves with wave length  $\lambda$  which equals to multiples of lattice parameter  $a$ , such as  $\lambda = a, 2a, 3a...$  corresponding to

$k = \frac{\pi}{a}, \frac{2\pi}{a}, \frac{3\pi}{a}...$  At these specific  $k$  vales the electron wave function

$$\begin{aligned} \psi_+ &\approx \exp(ikx) + \exp(-ikx) = 2 \cos(kx) \\ \psi_- &\approx \exp(ikx) - \exp(-ikx) = i2 \sin(kx) \end{aligned}$$

show strong or low interaction with atomic potential  $V$

resulting in the release of degeneration of electron energy- i.e. each energy value splits into two values

$$\begin{aligned} E(k)_+ &= \frac{\hbar^2}{2m} k^2 - V_+ \\ E(k)_- &= \frac{\hbar^2}{2m} k^2 + V_- \end{aligned}$$

resulting in an energy gap of  $E_g = V_- - V_+$ .

The presentation of allowed and forbidden electron energies as function of  $k$  is the extended zone scheme. The folding of all allowed states within an  $k$ -interval between  $-\frac{\pi}{a} < k < \frac{\pi}{a}$  is the reduced zone scheme. The filling of these bands determine the type of electric conductivity:

**Insulators** are solids with filled band separated by a large band gap energy to the next unfilled band. **Semiconductors** are similar to insulators, but  $E_g$  is in the order of  $kT$ , which allows few electrons to fill the upper empty level. **Metals** show large conductivity because one band is half filled, so electrons can find empty states within the same band.

**Density of state** The determination of energy states within the band structure which can be occupied by electrons can be performed in framework of quantum statistics → **density of states - DOS** → counts number of possible states per energy interval =  $dN/dE$

Number density is :  $n(E) = \frac{11.31\pi m^{3/2}}{h^3} \sqrt{E}$  independent of material used

Distribution of electrons on all these possible states is calculated using a distribution functions which considers electron spin and the Pauli-principle :

$n_{\text{besetzt}}(E) = n(E)p(E)$  mit  $p(E) = \frac{1}{\exp[(E - E_F)/kT] + 1}$  Fermi-Dirac-function

Occupation limit at  $T=0$  is the → Fermi energy  $E_F = \frac{h^2}{8m} \left( \frac{3n}{\pi} \right)^{2/3}$

For  $T=0 \rightarrow p(E) = 1$  für  $E \leq E_F$  and  $p(E)=0$  elsewhere.

For  $T>0$   $p(E)$  is changing only in close vicinity of  $E = E_F$ . A few electrons close below  $E_F$  get enough energy to occupy "free" closely above  $E_F$ .

**Electric conductivity:** only electrons close to  $E_F$  take place at the charge transport. Their

characteristic velocity is  $v_F = \sqrt{\frac{2E_F}{m}}$  → Fermi velocity, expressing the maximum velocity an electron can reach before scattering at another electron, defect, phonon aso.  $v_F \gg$  drift

velocity  $v_D = \frac{j}{(N_e - N_p)e}$   $N_e, N_p$  – concentration of electrons and holes, which is the real velocity of signal transport

Considering the specific band structure of a solid **electric conductivity,  $j$** , of metals and insulators or semiconductors are different  $j = \sigma E = ne\mu E$

Where  $\mu$  - is the mobility (Beweglichkeit) [ $\text{cm}^2/\text{Vs}$ ],  $n$  – number of „free“ charge carrier.

In metals  $n$  is constant (and high),  $\mu$  and  $j$  increase with decreasing the temperature or decrease with increasing the temperature due to the increase of scattering at thermally excited phonons and defects. Opposite for semiconductors, the conductivity increases for increasing temperature because more and more electrons are able to occupy states within the conduction band and can contribute to charge transport.