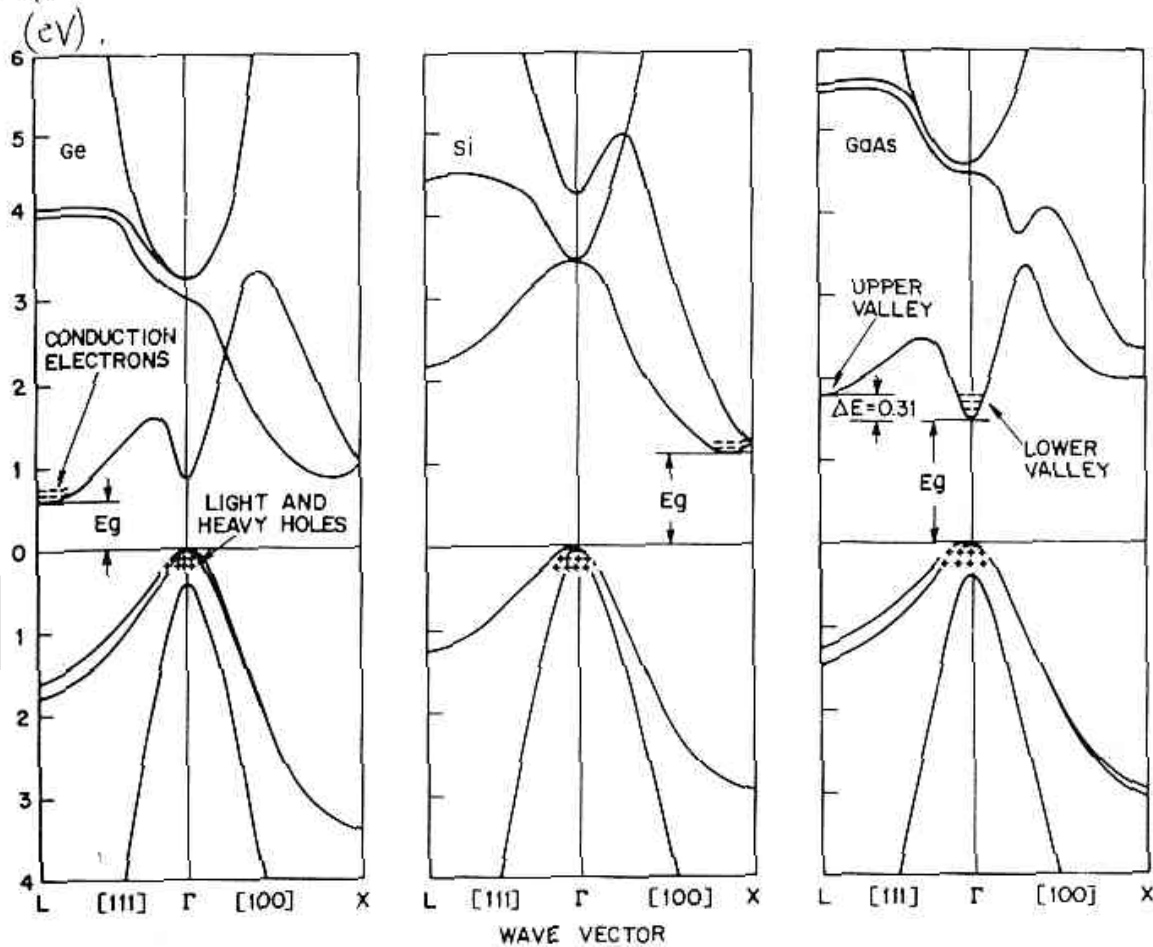
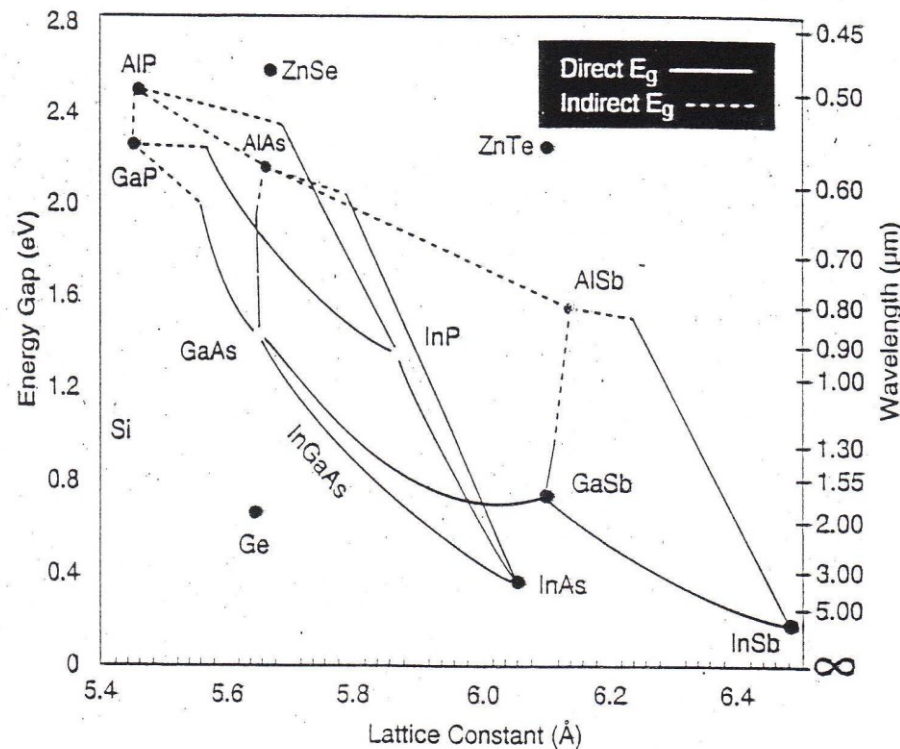


Energy Bands



. 5 Energy-band structures of Ge, Si, and GaAs, where E_g is the energy bandgap. s (+) signs indicate holes in the valence bands and minus (-) signs indicate electrons in the conduction bands. (After Chelikowsky and Cohen, Ref. 17.)

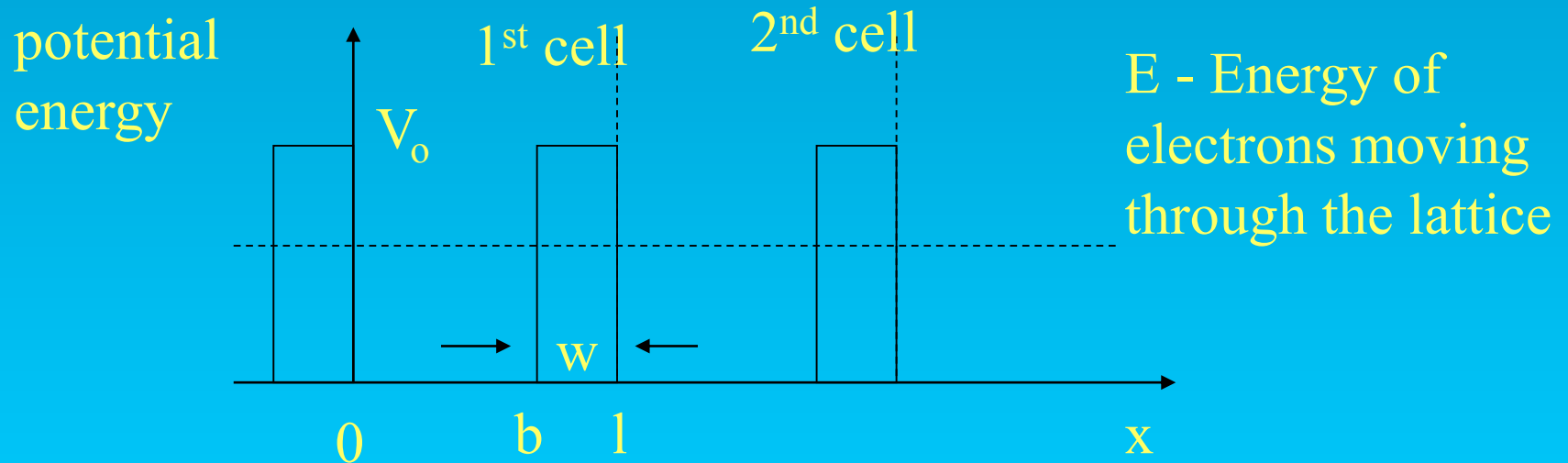
Rosetta Stone in Bandgap Engineering



- Effective mass
- Electron and hole mobility

Energy bands of electrons in solids

- Mathematical model of a solid (simple)



1D idealised model of an array of atoms in a solid –
Kronig-Penney model (square potentials)

- The potential experienced by an electron in the solid,

$$V(x) = V(x+nl)$$

$n = 1, 2, \dots$ For n atoms

Inside the wells, $V=0$ and for $0 \leq x \leq b$

$$\frac{\partial^2 \Psi}{\partial x^2} + \beta^2 \Psi = 0 \quad (1)$$

where

$$\beta^2 = \frac{2mE}{\hbar^2}$$

and in the barriers where $V_o > E$, for $b \leq x \leq l$,

$$\frac{\partial^2 \Psi}{\partial x^2} - \alpha^2 \Psi = 0 \quad (2)$$

where

$$\alpha^2 = \frac{2m(V_o - E)}{\hbar^2}$$

If we now let w , the width of the barrier go to zero and their height to infinity in such a way that the strength of the barrier, wV_o , remain constant i.e. the potential becomes a periodic delta function, the solution of which satisfies 1 and 2 is,

- $\psi = U_k(x) e^{jkx} \quad (3)$

- where $\lambda = 2\pi/k$, - a plane wave travelling in the +ve or -ve x direction depending on the sign of k, when the normal exponential time dependence is included. U_k is the Bloch function – a periodic function which varies with the same periodicity as that of the lattice l . Therefore, the solution to S equation consists of travelling waves which are modulated periodically in space.

- The solutions to 1 and 2 are

$$\psi(x) = Ae^{j\beta x} + Be^{-j\beta x} \quad \text{for } 0 \leq x \leq b$$

$$\psi(x) = Ce^{-\alpha x} + De^{\alpha x} \quad \text{for } b \leq x \leq l$$

Due to the periodicity of the potential,
applying (3)

$$\psi(x+l) = U(x+l)e^{j(x+l)k} = U(x) e^{jkx} e^{jkl}$$

For the 2nd cell, the solution becomes : (at 1)

$$\psi(x) = \{Ae^{j\beta(x-l)} + Be^{-j\beta(x-l)}\} e^{jkl}$$

Matching ψ at $x=b$

$$Ae^{j\beta b} + Be^{-j\beta b} = Ce^{-\alpha b} + De^{\alpha b}$$

Matching $d\psi/dx$ at $x=b$:

$$j\beta (Ae^{j\beta b} - Be^{-j\beta b}) = \alpha (-Ce^{-\alpha b} + De^{\alpha b})$$

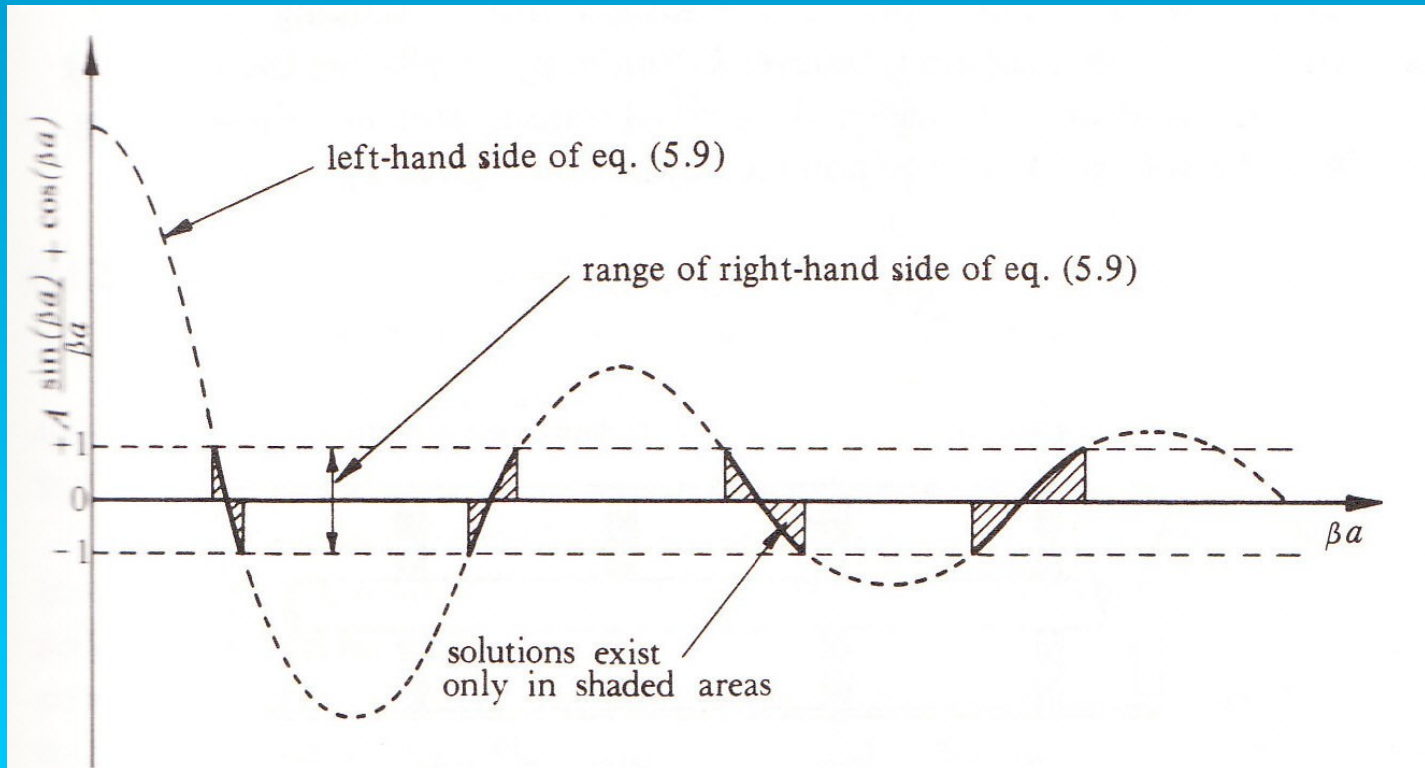
at $x=l$

$$\psi: Ce^{-\alpha l} + De^{\alpha l} = (A+B) e^{jkl}$$

$$d\psi/dx: \alpha(-Ce^{-\alpha l} + De^{\alpha l}) = j\beta (A-B)e^{jkl},$$

- Solving for A,B,C and D gives the solution for particular values of electron energy E, which satisfy:

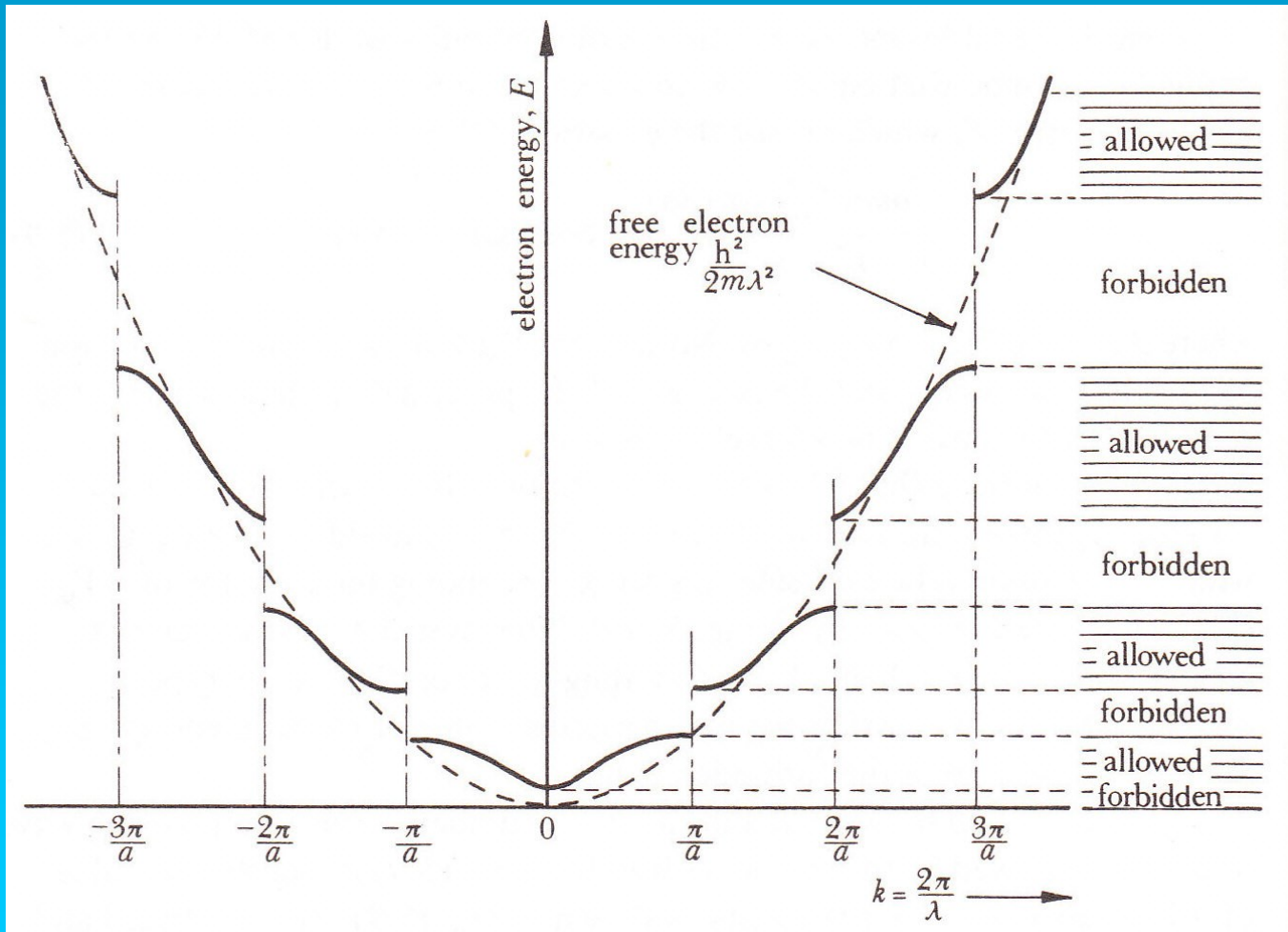
$$\left(\frac{mlwV_o}{\hbar^2} \right) \frac{\sin(\beta l)}{\beta l} + \cos(\beta l) = \cos(kl)$$



- Therefore, if the barrier strength is increased, i.e. wV_0 is made larger, the forbidden bands are widened.
- As $wV_0 \rightarrow 0$, (4) reduces to
- $\beta=k$ and $\beta=k = 2\pi/\lambda = \frac{\sqrt{2mE}}{\hbar}$

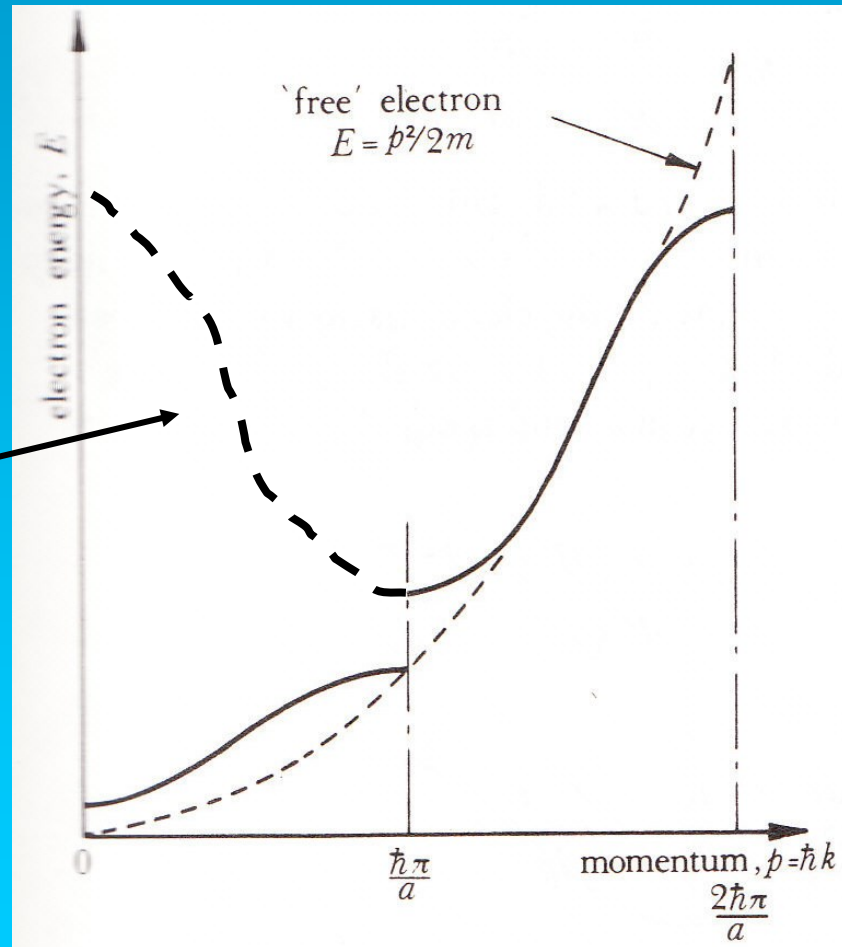
$$\Rightarrow E = \hbar^2/2m\lambda^2 \quad \text{free electron case}$$

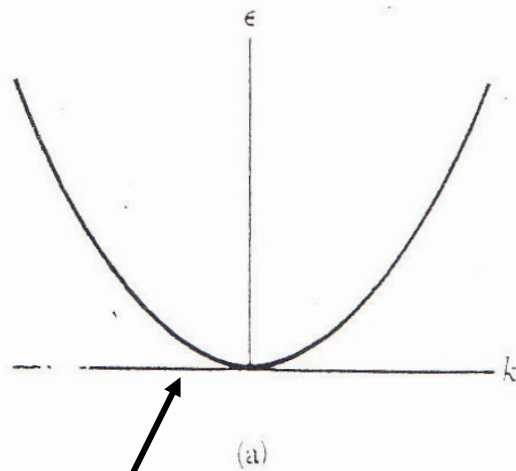
where electrons can move freely inside the solid.



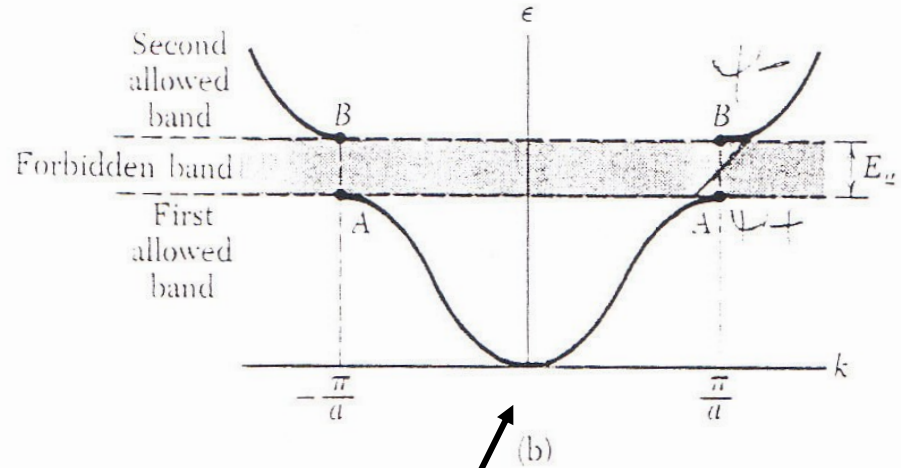
Energy vs Momentum

Reduced Zone Scheme





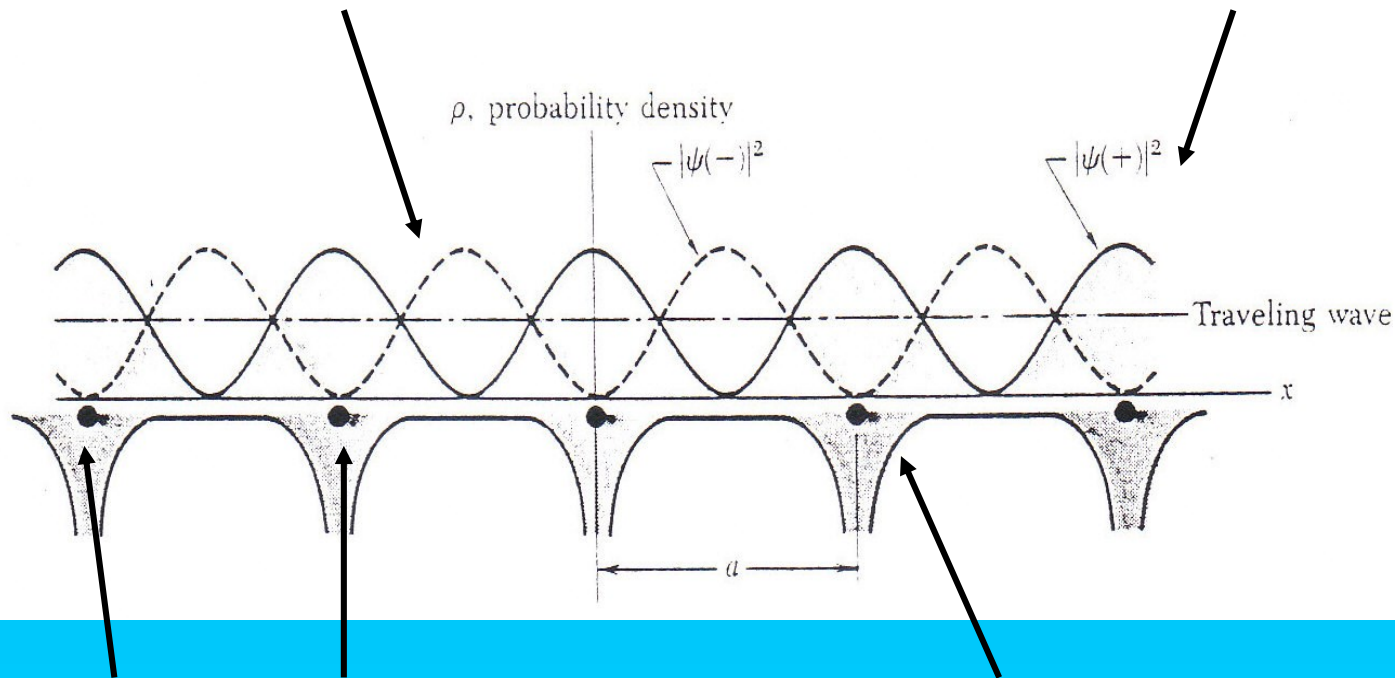
Plot of energy vs wavevector k for free electron



Plot of energy vs wavevector for an electron in a monatomic lattice of lattice constant a .

Wavefunction piles up electronic charge in the region between the positive ions, thereby raising the potential energy in comparison with the average potential energy seen by a travelling wave

Wavefunction piles up electronic charge on the cores of the positive ions, thereby lowering the potential energy in comparison with the average potential energy seen by a travelling wave



Ion cores

Potential energy

Velocity and effective mass of electrons in a solid

- For a free electron, its kinetic energy is related parabolically to p , its momentum,
- $p=mv$ and $E = p^2/2m$
- However, as we have seen, electrons in a solid are not free, they move under the combined influence of 1) an external field and 2) the periodic potential due to atom cores in the lattice \rightarrow gaps in their energy

- Now, an electron moving through the lattice can be represented by a wavepacket of plane waves grouped around some value of k , each wave component being of the form :

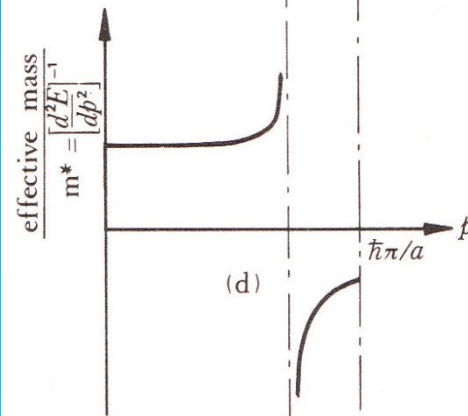
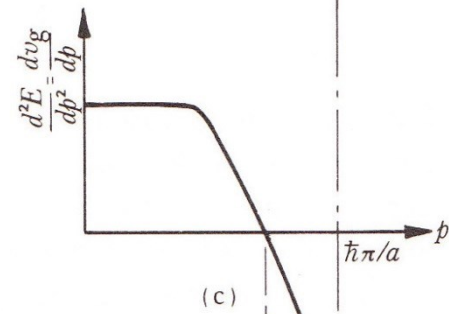
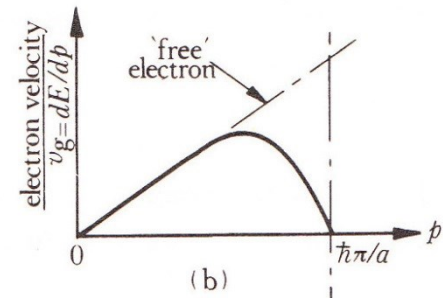
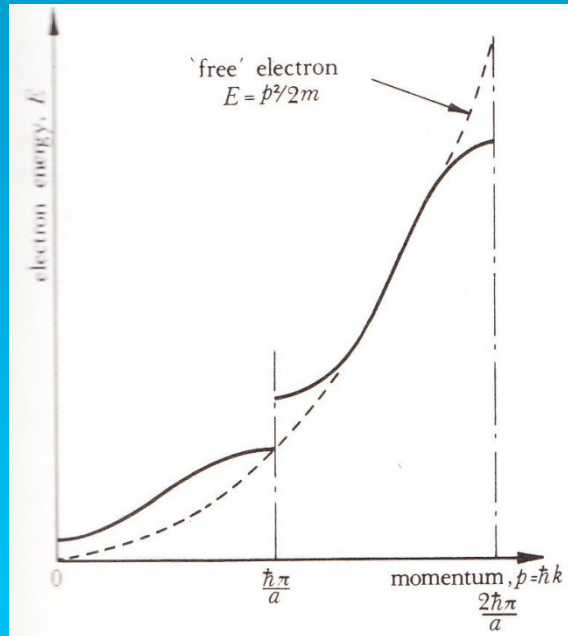
$$\exp - j \left[\frac{Et}{\hbar} - kx \right]$$

Therefore, the group velocity

$$v_g = \partial\omega/\partial k = \partial (E/\hbar)/\partial k = 1/\hbar \cdot \partial E/\partial k = \partial E/\partial p$$

Therefore, the velocity of an electron which is represented by a packet of waves centred near to a particular value of $k = k_0$ is proportional to the slope of the E-p or the E-k curve evaluated at k_0 .

Draw :



- The electron velocity $\partial E / \partial p$ falls to zero at band edges \Rightarrow the existence of standing waves $|\psi(-)|^2$ - ρ - probability density and $|\psi(+)|^2$ where the group velocity $v_g = 0$

Influence of an electric field

Now, consider an electronic wavepacket moving in a crystal lattice under the influence of an externally applied uniform E-field.

If the electron has an instantaneous velocity v_g and moves a distance δx in the direction of an accelerating force F , in time δt , it acquires energy:

$$\delta E = F \delta x = F v_g \delta t$$

$$\delta E = F / \hbar \cdot \delta E / \delta k \cdot \delta t$$

$$\Rightarrow dk/dt = F / \hbar \quad (1)$$

For a classically free electron, this is just

$$F = d(\hbar k)/dt = dp/dt = m dv/dt \quad (2)$$

However, taking into account of the forces associated with the periodic lattice potential, the acceleration of an electronic wavepacket in a solid is:

$$\text{Acceleration} = \frac{dv_g}{dt} = \frac{d}{dt} \left(\frac{dE}{dp} \right) = \frac{d^2 E}{dt dp}$$

$$\text{Or using (1)} \quad \frac{dv_g}{dt} = \frac{dp}{dt} \cdot \left(\frac{d^2 E}{dp^2} \right) = F \frac{d^2 E}{dp^2}$$

$$\Rightarrow F = \left(\frac{d^2 E}{dp^2} \right)^{-1} \cdot \frac{dv_g}{dt}$$

- Comparing this with (2) $\Rightarrow (d^2E/dp^2)^{-1}$ is a mass \rightarrow an effective mass for an electron moving in a periodic lattice of a solid

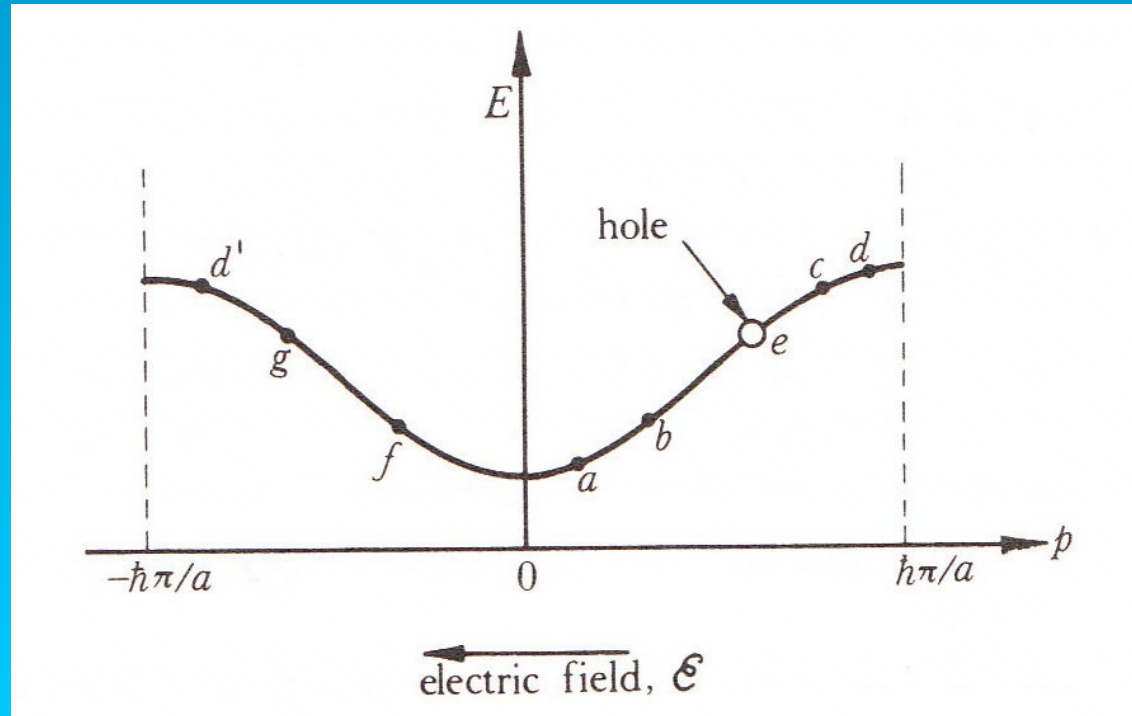
$$m^* = \left(\frac{d^2 E}{dp^2} \right)^{-1} = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1}$$

and $F = m^* dv_g/dt$

m^* is

- not a constant but is a function of energy
- can vary over a range from a few % to much greater than m
- at bottom of band, +ve effective mass \rightarrow electrons
- at top of band, -ve effective mass \rightarrow holes

- When e-field is impressed on electron, it will accelerate and move from a to b, where both its energy and velocity increases.
- However, at c, when the field is applied again, the electron moves to d, where its energy increases but its velocity decreases
→ an electron with –ve mass → hole → m_h^*



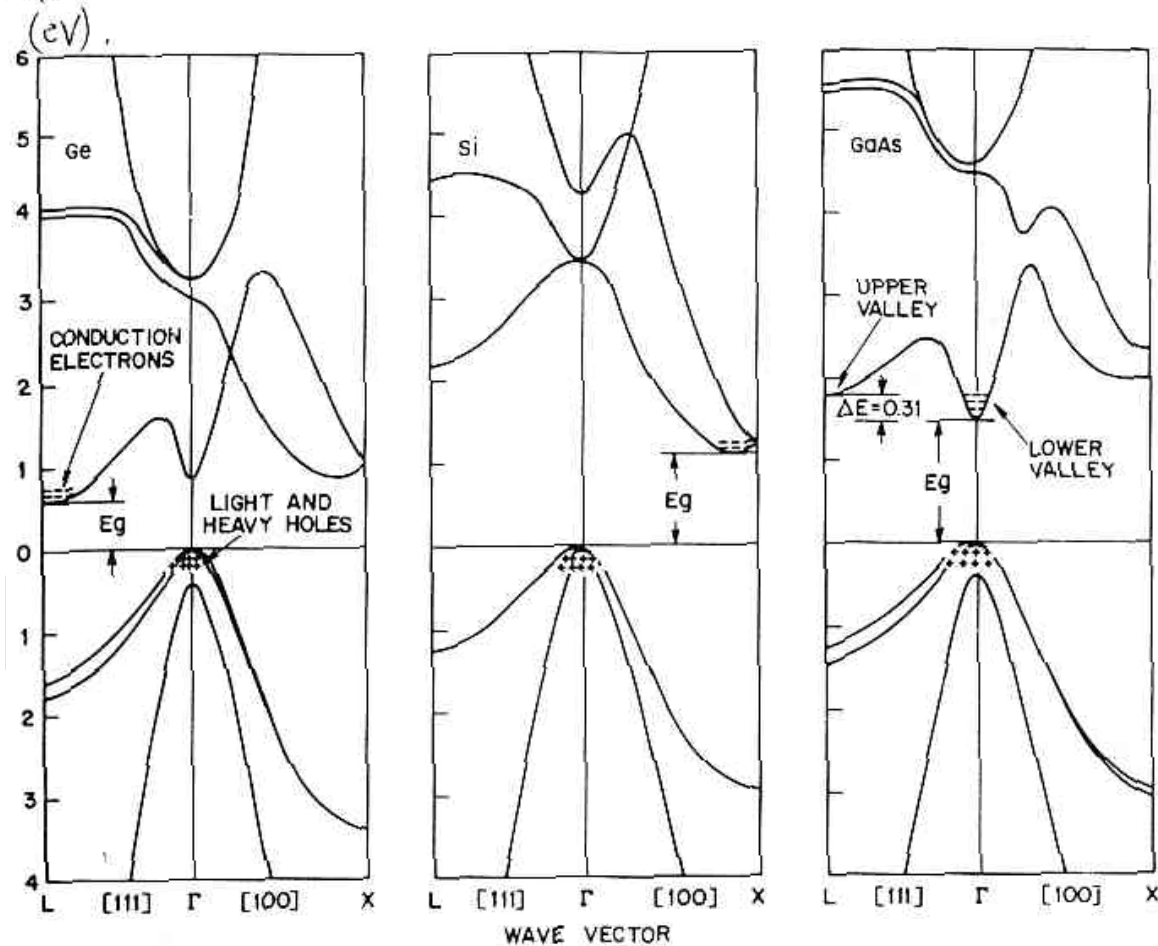
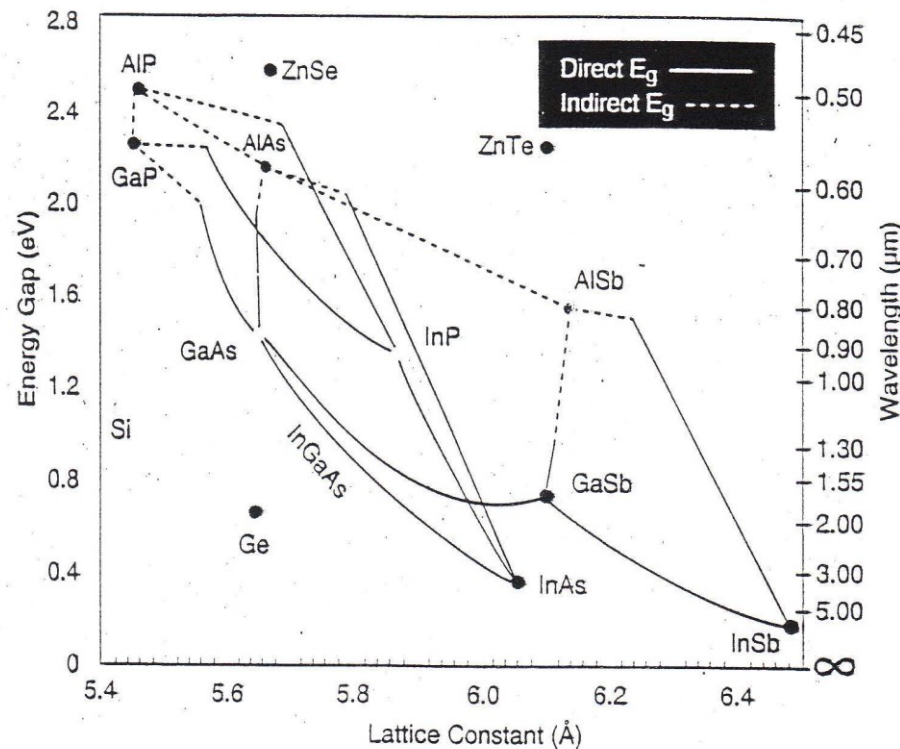


Figure 5. Energy-band structures of Ge, Si, and GaAs, where E_g is the energy bandgap. Plus (+) signs indicate holes in the valence bands and minus (-) signs indicate electrons in the conduction bands. (After Chelikowsky and Cohen, Ref. 17.)

Rosetta Stone in Bandgap Engineering



- Effective mass
- Electron and hole mobility

Electron transport

Free electron model,

$$J = \sigma E$$

where J is the current density, σ is the conductivity and E the electric field

Assume current flow due to n electrons, each of charge $-e$ and travelling at velocity v ,

$$J = -nev$$

Now, an electron subjected to an electric field E experiences an accelerating force $F = -eE$ and in the absence of scattering, the current density J would increase with time. This does not happen. Therefore, the electron velocity must remain constant for any applied field \rightarrow collisions, scattering.

A free electron can be accelerated from rest by the application of an external E-field, increases the velocity for a short time, then scatters and its velocity $\rightarrow 0$. Therefore, the electron acquires an average drift velocity v_d in the direction of the accelerated force, superimposed onto its random thermal motion.

If the average time between collisions is τ , the number of collisions/second is $1/\tau$ and the average rate of change of momentum (frictional force on carriers) due to the collision is mv_d/τ , the equation of motion of an electron subjected to an applied field in the x-direction E_x ,

$$-eE_x = m \frac{dv_{Dx}}{dt} + \frac{mv_{Dx}}{\tau}$$

The solution of this equation is

$$v_{Dx} = \frac{-e \tau E_x}{m \left(1 - e^{-\frac{t}{\tau}}\right)}$$

Therefore,

$$J = n(-e).v_{Dx} = \frac{ne^2 \tau E_x}{m \left(1 - e^{-\frac{t}{\tau}}\right)}$$

- We see that the electron drift velocity and the current density both rise exponentially with time to become a constant in a time comparable to τ .
- τ is the electron relaxation time, τ^{-1} is the scattering rate, therefore, scattering controls mobility.
- τ is $\approx 10^{-14}$ s and for any time after the application of the field longer than this \rightarrow steady state

$$v_D = \frac{-e\tau E}{m} = -\mu E$$

$$J = \frac{ne^2\tau E}{m}$$

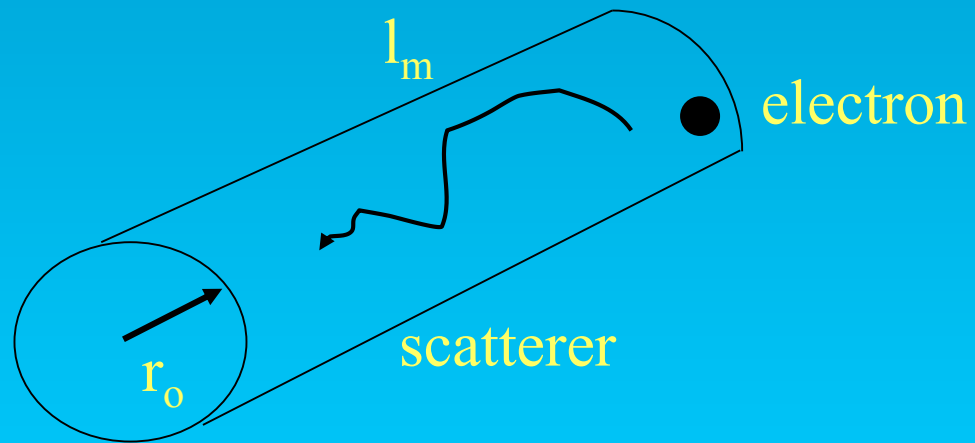
$$\mu = \frac{e\tau}{m}$$

- In the absence of scattering, the mean free path $l_m = \tau v$ of the electrons in the solid \rightarrow infinity
- scattering caused by thermal lattice vibrations, lattice defects, or the presence of impurity atoms and boundaries.
- lattice scattering \rightarrow thermally induced lattice vibrations, dominant at increasing temperatures
- impurity scattering \rightarrow ionised or otherwise, alter the local electrostatic potential. Its effect on deflecting the electron is greater when the electron is travelling slower. Therefore, impurity scattering tends to dominate in purer crystals at low temp., and when impurity concentration is high.

Impurity scattering

- Electrons scatter from donors and acceptors in semiconductors. Scattering centres have an aerial cross section S , seen by the electron. We can use this model to estimate the mean free path l_m .

Impurity scattering



An electron hits scatterer after distance l_m , so there is one impurity in the volume considered.

$$N_{\text{imp}} l_m S \approx 1$$

where N_{imp} is the number density of scatterers

$$\Rightarrow l_m \approx 1/S.N_{\text{imp}}$$

$$\text{now, } S = \pi r_o^2$$

where r_o is the effective radius

and for an ionised impurity, the potential acting on an electron

$$V(r) = \frac{e}{4\pi\epsilon_r\epsilon_o} \frac{1}{r}$$

And for an electron at $V(r_o)$.

The energy E of the electron

$$E = \frac{e^2}{4\pi\epsilon_r\epsilon_o} \frac{1}{r_o}$$

At r_o ,

$$S = \pi r_o^2 = \pi \left(\frac{e^2}{4\pi\epsilon_r\epsilon_o} \frac{1}{E} \right)^2$$

And $l_m = v\tau \Rightarrow \tau = l_m/v$ and $E = \frac{1}{2} mv^2$

$$\begin{aligned}
\mu &= \frac{e \tau}{m} = \frac{e}{m} \frac{1}{SN_{imp}} \frac{1}{v} \\
&= \frac{e}{m} \sqrt{\frac{m}{2E}} \frac{1}{N_{imp}} \frac{1}{\pi} \left(\frac{4\pi\epsilon_r \epsilon_o}{e^2} \right)^2 E^2 \\
&= e \left(\frac{E^{3/2}}{\sqrt{2m}} \right) \frac{1}{\pi} \frac{1}{N_{imp}} \left(\frac{4\pi\epsilon_r \epsilon_o}{e^2} \right)^2
\end{aligned}$$

From Boltzmann's distribution,

$$E \approx 3/2 k_B T$$

$$\mu \propto \frac{(kT)^{3/2}}{m^{1/2} N_{imp}}$$

=> as T increases, μ increases

In practice, μ decreases as temp. increases. This is because impurity scattering is less dominant at high temperatures \rightarrow more important at low temperatures

Phonon scattering

This becomes important at high temperature => more vibrations in the lattice

Acoustic phonons → like sound waves, compressive vibrations

Optical phonons → transverse lattice vibrations

Energy \ll electron, therefore quasi-elastic scattering

For phonon scattering, $1/\tau \propto T^{3/2}$

So, $\mu \propto T^{-3/2}$

Therefore, $1/\mu = m/e [1/\tau_{\text{imp}} + 1/\tau_{\text{phon}} + 1/\tau_{\text{e-e}} \dots]$

- Other mechanisms :
- Surface roughness e.g. GaAs/AlGaAs; Si/SiGe interface
- Alloy scattering – in SiGe
- Electron-electron scattering – at low temp.
- Intervalley scattering