EEE 6212
Semiconductor Materials

Lecture 25: Quantum confinement – the basics

Lecture 25: Quantum confinement

- density of states (DOS) in different dimensions
- particle in a box model with infinite barrier height
- excitons

density of states (DOS)

Density of states (DOS) describes the number of electronic states available in a system and is thus essential for calculating carrier concentrations and energy distributions of charge carriers in a semiconductor.
Depending on the dimensionality of the system, we need to distinguish

- 3D: bulk
- 2D: very thin layers ('quantum wells')
- 1D: very thin slabs (nanowires or 'quantum wires')
- 0D: very small particles, either epitaxial or colloidal 'quantum dots'

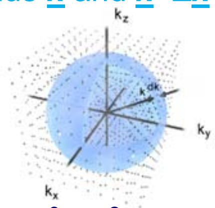
What means 'small'? -> of the order of the extent of the quantum mechanical wavefunction (1-5nm) or at least much smaller than the exciton size in semiconductors (3-15nm).

DOS in general dimensions

Scheme:
We need to calculate the number of allowed energy levels in k-space.
Consider particle with energy $E=p^2/(2m)=\hbar^2k^2/(2m)$, where $\underline{\mathbf{p}}=\hbar\underline{\mathbf{k}}$ describes the momentum for wavevector $\underline{\mathbf{k}}$ and m the mass. This parabolic band model yields $k=\sqrt{(2mE/\hbar^2)}$.
Differentiation yields $dk/dE=(2mE/\hbar^2)^{-1/2}\, m/\hbar^2$.
Assume all $\underline{\mathbf{k}}$-vectors are distributed evenly in k-space.
The number of states is then given by dividing the volume $V_{jD}dk$ of all states between $\underline{\mathbf{k}}$ and $\underline{\mathbf{k}}+\Delta\underline{\mathbf{k}}$ by the volume of a single state, v_{jD} ,multiplied by a factor of 2 for the spin as an additional degree of freedom:
$D(k)_{jD}\, dk = 2V_{jD}dk\, /v_{jD}$ (where j=dimensionality).
This then needs to be written as $D(E)dE$ in energy space, substituting k by $\sqrt{(2mE/\hbar^2)}$ and dk by $(2mE/\hbar^2)^{-1/2}\, m/\hbar^2\, dE$.

DOS in 3D

Consider volume of length L in real space of dimensionality 3. For $\underline{\mathbf{k}}=(k_x,k_y,k_z)=2\pi/L\ (n_x,n_y,n_z)$, where n_i are integer numbers, the volume of the unit cell in reciprocal space is $v_{3D}=(2\pi/L)^3$ and the space between the spheres of radius $\underline{\mathbf{k}}$ and $\underline{\mathbf{k}}+\Delta\underline{\mathbf{k}}$ is given by $V_{3D}dk=4\pi k^2\,dk$.



The number of states in k-space is then:

$D(k)_{3D}\,dk = 2V_{3D}dk\,/v_{3D} = k^2\,dk\,L^3/\pi^2$

Per unit volume we then get

$D(E)_{3D}\,dE= k^2\,dk\,/\pi^2 = 2mE/\hbar^2\,(2mE/\hbar^2)^{-1/2}\,m/\hbar^2\,1/\pi^2\,dE$

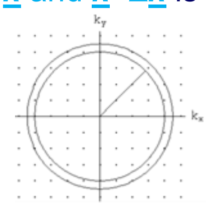
$= 1/(2\pi^2\hbar^3)\,(2m)^{3/2}\,E^{1/2}\,dE$

is proportional to $\sqrt{E}\,dE$

The 3D DOS is therefore a square-root function, similar to that of a free particle.

DOS in 2D

Consider volume of length L in real space for 2D system. For $\underline{\mathbf{k}}=(k_x,k_y,k_z)=(2\pi n_x/L,\ 2\pi n_y/L,\ k_z)$, where n_i are integer numbers, the volume of the unit cell in k-space is $v_{2D}=(2\pi/L)^2$ and the space between the rings of radius $\underline{\mathbf{k}}$ and $\underline{\mathbf{k}}+\Delta\underline{\mathbf{k}}$ is given by $V_{2D}\,dk=2\pi k\,dk$.



The number of states in k-space is then:

$D(k)_{2D}\,dk = 2V_{2D}dk\,/v_{2D} = 1/\pi\ k\,dk\,L^3$

Per unit volume we then get

$D(E)_{2D}\,dE= 1/\pi\ k\,dk\ = 1/\pi\ \ (2mE/\hbar^2)^{1/2}\,(2mE/\hbar^2)^{-1/2}\,m/\hbar^2\,dE$

$= m/(\pi\hbar^2)\,dE$

is constant and does no longer depend on E.

Immediately, as the top of the band-gap is reached, there are many available states. Taking also into account lower energy levels, the 2D DOS is a staircase of step functions.

DOS in 1D

Consider volume of length L in real space for 1D system. For $\underline{\mathbf{k}}=(k_x,k_y,k_z)=(2\pi n_x/L,\ k_y,\ k_z)$, where n is an integer, the volume of the unit cell in k-space is $v_{1D}=2\pi/L$ and the space between the end points of a line from $\underline{\mathbf{k}}$ to $\underline{\mathbf{k}}+\Delta\underline{\mathbf{k}}$ (and $-\underline{\mathbf{k}}$ to $-\underline{\mathbf{k}}+\Delta\underline{\mathbf{k}}$ for symmetry) is given by $V_{1D}\,\mathrm{d}k=2\,\mathrm{d}k$.

The number of states in k-space is then:
$D(k)_{1D}\,\mathrm{d}k = 2V_{1D}\mathrm{d}k\,/v_{1D} = 2/\pi\ \mathrm{d}k\ L^3$
Per unit volume we then get
$D(E)_{1D}\,\mathrm{d}E = 2/\pi\ \mathrm{d}k\ = 2/\pi\,(2mE/\hbar^2)^{-½}\ m/\hbar^2\,\mathrm{d}E$
$= (2m)^{½}/(\pi\hbar)\ E^{-½}\,\mathrm{d}E$
has a form similar to the branch of a hyperbola.
Taking into account lower energy levels, the 1D DOS is a staircase of such branches stacked on top of each other.

DOS in 0D

All values of $\underline{\mathbf{k}}$ are quantised in all three directions in k-space , as no free motion is possible in real space.
There is hence no continuous k-space to be filled and all available states exist only at discrete energies, so the DOS in 0D for electrons can be described by a delta function (again, with a factor 2 for the spins):
$D(E)_{0D}\,\mathrm{d}E = 2\ \delta(E-E_c)$
is a delta-function. Taking into account lower energy levels, the 0D DOS is a series of delta functions.

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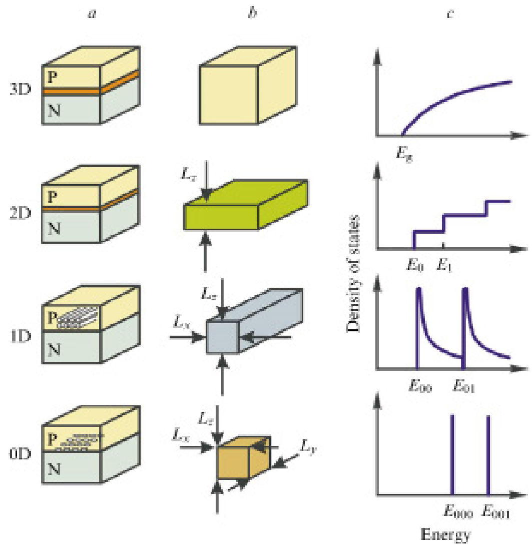
DOS overview, part I



type of confinement

none

a potential well or quantum well confines particles to movement in (x,y) plane

a quantum wire or nano-rod confines particles to movement along y-direction only

total confinement by quantum dot: particle can no longer move at all.

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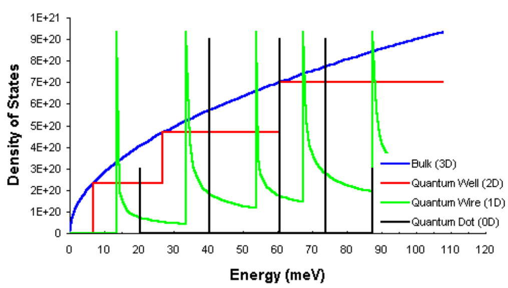
DOS overview, part II

The stronger the confinement is, the more the initially continuous DOS splits up into discrete levels. This means a narrower range of wavelengths in optical emission or absorption, which is useful for opto-electronics.



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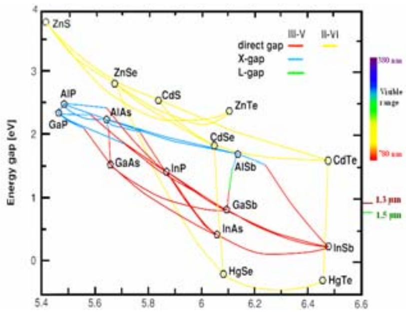
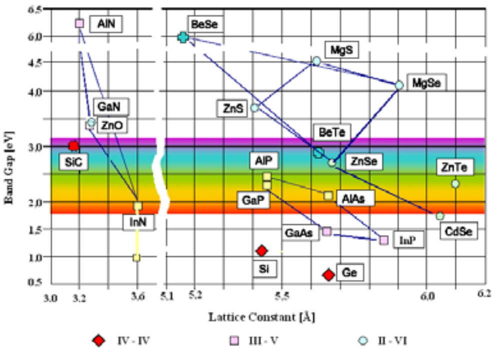
semiconductor band-gaps

The spontaneous and stimulated emission processes are vastly more efficient in direct band-gap semiconductors than in indirect band-gap semiconductors; therefore GaAs rather than Si is commonly used for laser diodes.





source: U Kiel

model: particle in a box with infinite barrier height

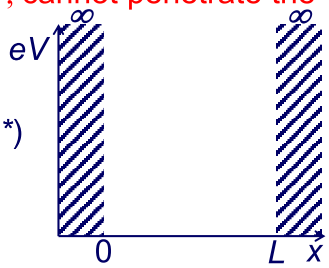
Consider the Schrödinger equation for a particle of effective mass m^* in a box of length L with infinitely high barriers along *x at positions* 0,L. The wavefunction, Ψ, cannot penetrate the infinitely high barrier, so:

$-\hbar^2/(2m^*)\, \nabla^2\, \Psi = E\, \Psi$ with $\nabla^2 = \partial^2/\partial x^2$

With common Ansatz and $E = \hbar^2 k^2/(2m^*)$

$\Psi(x) = A \exp(+jkx) + B \exp(-jkx)$

$\quad = (A+B) \cos kx + j\,(A-B) \sin kx$



If the particle is described by a standing wave in the box so that $L = n\,\lambda/2$, n an integer, then $k = 2\pi/\lambda = n\pi/L$. Quantisation of $\underline{\boldsymbol{k}}$ gives discrete energy levels:

$E_n = \hbar^2/(2m^*)\, (n\pi/L)^2$, n=±1,2,3,…

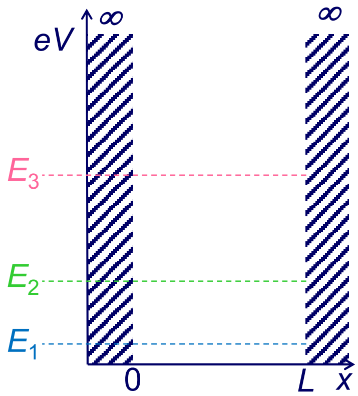
model: particle in a box with infinite barrier height

$\Psi(x)$= A exp(+jkx) + B exp(−jkx)

= (A+B) cos kx + j (A−B)sin kx

For the boundary conditions $\Psi(x=0)=0=\Psi(x=L)$, we get A+B=0, so only the sine-terms remain.

Also need $\int_0^L |\Psi(x)|\,dx=1$ for a normalised wavefunction; this will give $\Psi_n=C_n \sin(n\pi x/L)$ where the pre-factors C_n will depend on n.



$E_1=\hbar^2/(2m^*)\,(\pi/L)^2$

$E_2=\hbar^2/(2m^*)\,(2\pi/L)^2$

$E_3=\hbar^2/(2m^*)\,(3\pi/L)^2$

Note $E_n \propto (n/L)^2$

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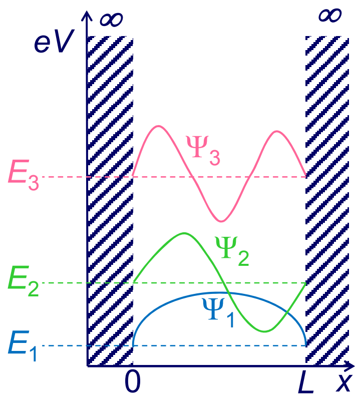


The wavefunction Ψ_n shows n half cycles of the sine function.

electron-hole pair in a type-I quantum well with very high barriers

Both electron and hole are confined within the quantum well, with ground states for n=1 of

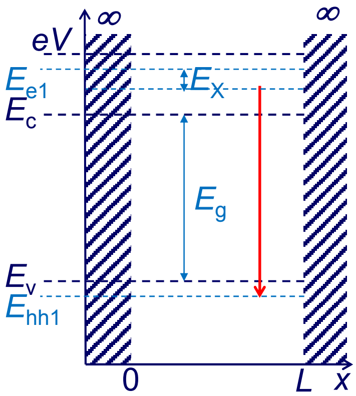
$E_{e1}=\hbar^2/(2m_e^*)\ (\pi/L)^2$ for electron and

$E_{hh1}=\hbar^2/(2m_{hh}^*)\ (\pi/L)^2$ for heavy hole.

The pair also attract each other by Coloumb attraction and form a so-called exciton of binding energy E_x.

The energy of a PL emission line then is:

$E_{PL}=E_g+E_{e1}+E_{hh1}-E_X$



electron-hole pair in a type-I quantum well with very high barriers

$E_{PL}=E_g+E_{e1}+E_{hh1}-E_X$

Example for a 10nm InAs QW in GaAs:

E_g=0.354eV

E_x=0.022eV

$m_e=0.023m_0$ -> $E_{e1}=\hbar^2/(2m_e^*)(\pi/L)^2$=0.163eV

$m_{hh}=0.41m_0$ -> $E_{hh1}=\hbar^2/(2m_{hh}^*)(\pi/L)^2$=0.009eV

then:

$E_{PL}\approx$ (0.354+0.163+0.009-0.022)eV=0.504eV

is still IR (λ=2.46μm) but significantly higher in energy (i.e. blue shifted) compared to pure band-edge luminescence in bulk InAs!

For more detailed calculation: need FINITE well depth, which results in

a) the wavefunction leaking into the barrier material by typically ~1nm and

b) reduces the confinements energies.