Condensed Matter Physics: Important Concepts

- crystal structure of Si, Ge, GaAs, III-V’s
- semiconductor bandstructure
- effective mass approximation
- valence bands and spin-orbit coupling
- density of state
- doping
Condensed Matter Physics: Important Concepts

Silicone (Si)

diamond structure of Si

face centered cubic lattice
two atomic base: (0,0,0) and (a/4, a/4, a/4)

a = 5.65 Å

brillouin zone (bcc)

column IV material

Ge also has diamond structure
Gallium Arsenide (GaAs)

zincblende structure of GaAs

dito Si, but one atom Ga, one As

a = 5.43 Å

brillouin zone (bcc)

III – V semiconductor (binary compound)
III-V binaries
zinc-blende

II-VI binaries, also zinc-blende
Electrons obey the Schrödinger equation (neglecting interaction)

\[
\left\{ \frac{-\hbar^2}{2m} \Delta + V(\vec{r}) \right\} \psi(\vec{r}) = \varepsilon \psi(\vec{r}) \quad (1)
\]

\( \psi(\vec{r}) \): wave function

\( V(\vec{r}) \): periodic potential \( U(\vec{r} + \vec{R}) = U(\vec{r}) \)

Free electrons: \( V = 0 \) \( \Rightarrow \) \( E = \frac{\hbar^2 k^2}{2m} \) \( \psi = e^{i \beta \vec{k} \cdot \vec{r}} \) plane wave

\( \rightarrow \) parabolic dispersion
in periodic potentials,

periodically, Bloch theorem:

\[ \psi(r) = \psi_k(r) = e^{i k \cdot r} u_k(r) \]  \hspace{1cm} (2)

with\[ u_k(r+R) = u_k(r) \] \hspace{1cm} (3)

put (2) in (1), get

\[ \frac{\hbar^2}{2m} \left( -i \nabla + k \right)^2 + U(r) \right) u_k(r) = \varepsilon_k u_k(r) \] \hspace{1cm} (4)

with periodic boundary conditions. (3)

Eigenvalue problem. finite size: discrete spectrum, energy bands: \( \varepsilon_n(k) \)
k: limited to first Brillouin zone

\( \varepsilon_k = \varepsilon_{n,k} \) \hspace{1cm} \psi = \psi_{nk}(r)

metals, semiconductors, insulators...
metals, semiconductors, insulators…

exact solution usually impossible, but approximations exist.

Si (covalent): indirect gap
GaAs (polar): direct gap

momentum mismatch for photons
optically active

Si band structure
Ge band structure

- $E_g = 0.66$ eV
- $E_X = 1.2$ eV
- $E_{\Gamma_1} = 0.8$ eV
- $E_{\Gamma_2} = 3.22$ eV
- $\Delta E = 0.85$ eV
- $E_{\sigma_0} = 0.29$ eV
GaAs band structure

300 K
- $E_g = 1.42 \text{ eV}$
- $E_L = 1.71 \text{ eV}$
- $E_X = 1.90 \text{ eV}$
- $E_{so} = 0.34 \text{ eV}$
Fig. 3.14 Constant-energy surfaces characterizing the conduction-band structure in (a, d) Ge, (b) Si, and (c) GaAs. (d) shows the truncation of the Ge surfaces at the Brillouin-zone boundaries. [(a-c) after Sze and Ziman; (d) from McKelvey. Reprinted with permission; the latter from Robert E. Krieger Publishing Co., Malabar, Florida.]
Effective mass approximation
Valence bands

built from atomic p states
3 fold orbital degeneracy plus spin: degeneracy 6

spin-orbit coupling: relativistic effect (Dirac equation)
motion of electron in electric field: Lorentz transformation gives magnetic field component: couples to spin via Zeeman term

\[ H_{SO} = \frac{\hbar}{4m^2c^2} \vec{\sigma} \cdot \vec{\nabla}V \times \vec{p} \]

in spherically symmetric potential

\[ H_{SO} \sim \vec{L} \cdot \vec{S} \]

assume electrons in solid behave as individual atoms:
p-states: L=1, S=1/2
Valence bands (2)

p-states: L=1, S=1/2
addition of angular momenta

\[
1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}
\]

\[
\text{degeneracy} \quad 3 \times 2 = 4 + 2
\]

this gives
heavy/light hole bands (4)
split bands (2) lowered by \(E_{so}\)

\(E_{so}\) spin-orbit strength ~ local electric field of atom on site ~ nuclear charge \(Z\)

\(\begin{align*}
E_{so} & \sim 6 \text{ meV} & \text{graphite} \\
 & \sim 45 \text{ meV} & \text{Si} \\
 & \sim 340 \text{ meV} & \text{GaAs}
\end{align*}\)
GaAs band structure

300K $E_g = 1.42$ eV
$E_L = 1.71$ eV
$E_X = 1.90$ eV
$E_{so} = 0.34$ eV
Valence bands (3)

dispersion of the remaining bands
“k·p” approximation (around minima / maxima)

\[
\left\{ \frac{t_n^2}{2m} \left( -i \nabla + k \right)^2 + U(r) \right\} u_k(r) = \sum_{k} u_{k}(r)
\]

write out \((\ )^2\) and replace \(-i \partial\) with \(p\) (\(p\): operator, \(k\): number)

\[
\left[ \frac{p^2}{2m} + \frac{\hbar \vec{k} \cdot \vec{p}}{m} + \frac{\hbar^2 k^2}{2m} + V(r) \right] u_{n,k}(\vec{r}) = E_{n,k} u_{n,k}(\vec{r})
\]

treat \(k\cdot p\) term perturbatively….

different masses: light and heavy holes, but degenerate at \(k=0\)

hole masses: negative \hspace{1cm} hole charge: negative \hspace{1cm} positive transport (q/m)
Valence bands (4)

hole masses
Si $m_{HH}^* = 0.54 \, m_e$
  $m_{LH}^* = 0.15 \, m_e$
GaAs $m_{HH}^* = 0.51 \, m_e$
  $m_{LH}^* = 0.08 \, m_e$

(vs. GaAs electron mass 0.067 $m_e$)
Replace fraction $0 \leq x \leq 1$ with Aluminium (Al): $\text{Al}_x\text{Ga}_{1-x}\text{As}$

![Graph showing 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).](image.png)
Occupation of bands

electronic density of states \( D_d(E) \)

# of states available in a window of energy \([E, E+dE]\).
d : dimensionality of the system

periodic boundary conditions (cube, square, line) of length \( L \) (endresult independent of \( L \))

\[
\psi (\vec{r} + (L, L)) = \psi (\vec{r})
\]
Electronic Density of States

\[ D_1(E) = \frac{g \sqrt{2m}}{2\pi \hbar} \cdot \frac{1}{\sqrt{E}} \]

\[ D_2(E) = \frac{gm}{2\pi \hbar^2} \quad \text{independent of energy} \]

\[ D_3(E) = \frac{g (2m)^{3/2}}{4\pi^2 \hbar^3} \cdot \sqrt{E} \]

plus Fermi-Dirac distribution gives carrier occupation…
Doping

Control mobile carrier type (n or p) and density by implanting dopants donors (give off electron) or acceptors (take in electron)

example replace Ga (3 valence electron) with Si (4 valence electrons)
    1 extra electron (plus a proton left behind)

similar to a hydrogen atom in a medium with dielectric constant $\varepsilon_{\text{GaAs}} \sim 13$

\[
\left[ -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r} \right] \psi(r) = [E - E_C] \psi(r)
\]

(envelope wave function $\psi$ varies slowly compared to unit cell)

\[ E_{\text{DOPANT}} = E_C - 13.6 \text{ eV} \frac{m^*}{\varepsilon^2 m_e} \quad \frac{m^*}{\varepsilon^2 m_e} \sim \frac{1}{2500} \]

binding energy $\sim 5.4$ meV

Bohr radius: $a_B^* = \frac{\varepsilon}{m_e} a_B \sim 10.3 \text{ nm} \gg 5.4 \text{ Å}$

atomic Bohr radius: 0.53 Å