Outline

- Miller Indices of a Crystal
- Band Structure of a Crystal – Notations of Wavevector $\mathbf{k}$
- Indirect vs. Direct Bandgaps
- $\mathbf{k} \cdot \mathbf{p}$ Theory for Band Structure Calculation
- Quantum Well Lasers – how does NANO help here?
Miller indices

- Miller indices – a notation to describe planes and directions in a crystal.

- \([h \ k \ l]\) – denotes a direction.
- \(<h \ k \ l>\) – denotes equivalent directions. E.g., in cubic system, \(<1 \ 0 \ 0>\) denotes \([1 \ 0 \ 0], [0 \ 1 \ 0], [0 \ 0 \ 1]\) and their negative directions.
- \((h \ k \ l)\) – denotes a set of parallel planes. In cubic system, it means that the plane is normal to \([h \ k \ l]\) direction.
- \{h k l\} – denotes equivalent planes. E.g., in cubic system, \{1 0 0\} denotes \(1 0 0), (0 1 0), (0 0 1)\) planes.

How to index a plane?

- Reference: http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm

- **Step 1**: *Identify the intercepts on the x-, y- and z- axes.*
- **Step 2**: Specify the intercepts in fractional co-ordinates.
- **Step 3**: Take the reciprocals of the fractional intercepts.
Example

1. The (110) surface

Assignment
Intercepts: a, a, 0
Fractional intercepts: 1, 1, 0
Miller Indices: (110)

http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm

Example

* Semiconductor nanowires tend to grow along <111> directions!

2. The (111) surface

Assignment
Intercepts: a, a, a
Fractional intercepts: 1, 1, 1
Miller Indices: (111)

http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm
Example

{1 0 0} planes in cubic systems

- Equivalent planes

Assignment

Intercepts: $\frac{1}{2}a, \infty, \infty$

Fractional intercepts: $\frac{1}{2}, 1, \infty$

Miller Indices: (110)

http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm
Si Band Structure – Indirect Bandgap

\[ \Gamma: \mathbf{k} = 0 \]
\[ \chi: \mathbf{k} = [100] \frac{2\pi}{a} \]
\[ L: \mathbf{k} = [111] \frac{2\pi}{a} \]
\[ K: \mathbf{k} = [110] \frac{2\pi}{a} \]

from: Yu & Cardona – Fundamentals of Semiconductors

GaAs Band Structure – Direct Bandgap

from: Yu & Cardona – Fundamentals of Semiconductors
Optical Transitions

- Photon: large $E$, negligible $k$ (vertical transition)
- Phonon: small $E$, large $k$ (nearly horizontal transition)


Si can still be a good photodetector

- But not an emitter

Very fast relaxation to the X valley – no chance for e-h recombination unless assisted by a phonon.

from: Yu & Cardona – Fundamentals of Semiconductors
**Bloch’s Theorem**

A **Bloch wave** or **Bloch state**, named after Felix Bloch, is the wavefunction of a particle (usually, an electron) placed in a periodic potential. It consists of the product of a plane wave and a periodic function (Bloch envelope) $u_{nk}(r)$ which has the same periodicity as the potential:

$$\psi_{nk}(r) = e^{i \mathbf{k} \cdot \mathbf{r}} u_{nk}(r).$$

The result that the eigenfunctions can be written in this form for a periodic system is called **Bloch’s theorem**.

$e^{i \mathbf{k} \cdot \mathbf{r}}$: plane wave

$u_{nk}(r)$: periodic function

$$u_{nk}(r+ \mathbf{R}) = u_{nk}(r)$$


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**k ⋅ p Theory for Band Structure Calculation**

Consider the general Schrödinger equation for an electron wavefunction $y_{nk}(r)$ in the $n$th band with a wave vector $k$,

$$\left(\mathbf{p}^2 / 2m_0 + V(r) \right) y_{nk}(r) = E_n(k) y_{nk}(r)$$

(4.1.A)

When written in terms of $u_{nk}(r)$, it becomes

$$\left[ \frac{p^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + V(r) \right] u_{nk}(r) = \left[ E_n(k) - \frac{\hbar^2 k^2}{2m_0} \right] u_{nk}(r)$$

(4.1.5)

The above equation can be expanded near a particular point $k_0$ of interest in the band structure. When $k_0 = 0$, the above equation is expanded near $E_n(0)$.

**Equation for $u_{nk}(r)$**

$$\left[ H_0 + \frac{\hbar^2}{m_0} \mathbf{k} \cdot \mathbf{p} \right] u_{nk}(r) = \left[ E_n(k) - \frac{\hbar^2 k^2}{2m_0} \right] u_{nk}(r).$$

(4.1.5)

$$H_0 = \frac{p^2}{2m_0} + V(r)$$

$$E_n(k) = E_n(0) u_{nk}(r)$$

(4.1.7b)

from: S. L. Chuang – Physics of Optoelectronic Devices
**k • p Theory for Band Structure Calculation**

- Treat $k \neq 0$ as perturbation
- Good approximation for small $k$

\[
\begin{bmatrix}
H_0 + \frac{\hbar^2}{m_0} k \cdot p
\end{bmatrix} u_{nk}(r) = \left[ E_n(k) - \frac{\hbar^2 k^2}{2m_0} \right] u_{nk}(r) \tag{4.1.5}
\]

\[
H_0 = \frac{p^2}{2m_0} + V(r) \tag{4.1.7a}
\]

\[
H_0 u_{n0}(r) = E_n(0) u_{n0}(r) \tag{4.1.7b}
\]

from: S. L. Chuang – Physics of Optoelectronic Devices

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**k • p Theory for Band Structure Calculation**

- Including the Spin-Orbit Interaction

\[
H_{nk}(r) = \left( H_0 + \frac{\hbar^2}{m_0} k \cdot p + \frac{\hbar}{4m_0^2c^2} \nabla \times p \cdot \sigma \right) u_{nk}(r) = E u_{nk}(r) \tag{4.2.7}
\]

- Use the solutions for a hydrogen atom as $E(0)$ & $u_{n0}$
- Solve for $E(k)$
- Solve for $u_{nk}$
- Result: C, HH, LH, SO bands

from: S. L. Chuang – Physics of Optoelectronic Devices
**k • p Theory for Band Structure Calculation**

- Including the Spin-Orbit Interaction
- Result:

![Band structure diagram](image)

Figure 4.4. The band-edge energies $E_p$, $0$, and $-\Delta$ for the conduction, heavy-hole, light-hole, and spin split-off bands with their corresponding band-edge Bloch functions. Note that the dispersion relation $E \sim k$ for the heavy-hole band $E_{hh}$ should curve down as shown and follow the result of the Luttinger-Kohn model.

From: S. L. Chuang – Physics of Optoelectronic Devices

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**Quantum-Well Lasers**

- Workhorse for the semiconductor laser industry.
- Why quantum well?

1. Tunable wavelength (QW width)
2. Smaller threshold current (description see later slides)
3. etc...

![Bandgap profile](image)

Figure 10.16. Bandgap profiles for (a) single-quantum-well, (b) multiple-quantum-well, and (c) graded-index separate-confinement heterostructure (GRINSCH) semiconductor laser.

From: S. L. Chuang – Physics of Optoelectronic Devices
Recall: Density of States

- # of states per unit energy interval per unit volume
- Area bound below is the number of electrons filled up to a certain energy $E$ (times 2 to include spin)

Absorption

- Absorption curve is proportional to DOS curve (when $T=0$)

from: S. L. Chuang – Physics of Optoelectronic Devices
Gain

- Population Inversion
- Stimulated Emission
- Gain curve is proportional to DOS curve up to $F_c - F_v$ along the E axis (when $T=0$)

Negative absorption = Gain

from: S. L. Chuang – Physics of Optoelectronic Devices

Laser Lasing Requirement

- Gain = All the losses in the laser cavity

Energy $E = h\omega$

Lots of carriers required! (large threshold current)  
Very few carriers required. (smaller threshold current)