2. Intrinsic semiconductors
Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

Many important materials (silicon, steel) are crystals

Crystal Structure

Gallium crystals    quartz    Insulin crystals
Crystalline Structures

- **face centered cubic, fcc**
- **body centered cubic, bcc**
- **simple cubic**

The image illustrates the concept of Bravais lattices and how they form different crystal structures through the addition of a basis.
Crystal planes and directions: Miller indices

A plane with the intercepts $1/h$, $1/k$, $1/l$ is the $(h,k,l)$ plane.

[ ] specific direction
<> family of equivalent directions
() specific plane
{} family of equivalent planes

MOSFETs are made on <100> wafers.
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms in the conventional unit cell. (The image can be rotated with a mouse.)

Silicon surfaces

Si(100)

Si(111)

(Source: Sandia Nat.Labs.)
KOH etches Si \{110\} > \{100\} > \{111\}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

http://www.ece.uncc.edu/research/clean_room/fabprocesses/KOH-EtchingAndDecon.pdf
<table>
<thead>
<tr>
<th>Crystal structures</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Face Centered Cubic</td>
<td>Body Centered Cubic</td>
<td>Hexagonal Close Packed</td>
</tr>
<tr>
<td>Al, Cu, Ni, Ag, Pt, Au, Pb</td>
<td>W, Cr, Fe, Mo, Ta</td>
<td>Ti, Co, Zn, Zr</td>
</tr>
<tr>
<td>Diamond</td>
<td>Zincblende</td>
<td>Wurzite</td>
</tr>
<tr>
<td>C, Si, Ge, α-Sn</td>
<td>GaAs, InP, GaP, InAs, AlAs</td>
<td>ZnO, GaN, AlN, CdSe</td>
</tr>
</tbody>
</table>
face centered cubic (fcc)

Al, Cu,
Ni, Ag,
Pt, Au,
Pb

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc_jsmol.php
hexagonal close pack (hcp)

Ti, Co, Zn, Zr,

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/hcp/hcp_jsmol.php
Close packing

HCP = Hexagonal close pack
Hexagonal Bravais lattice with two atoms in the basis.
body centered cubic  bcc

W
Cr
Fe
Mo
Ta

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/bcc/bcc_jsmol.php
zincblende

ZnS
GaAs
InP
GaP
InAs
AlAs

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/zincblende/zincblende_3smol.php
wurtzite

ZnO
CdS
CdSe
GaN
AlN

Structural phase transitions

GaAs, Zincblende

GaAs, Wurtzite

3C - SiC

4H - SiC

6H - SiC

SiC has about 100 polytypes
Electrons

Charge = $-1.6022 \times 10^{-19}$ C
Mass = $9.11 \times 10^{-31}$ kg
Radius = ?

0.15 nm
Quantum Mechanics

Everything moves like a wave but exchanges energy and momentum like a particle.

www.almaden.ibm.com/vis/stm/atomo.html
Everything moves like a wave but exchanges energy and momentum like a particle.
de aangegeven golflengten gelden in vacuüm

<table>
<thead>
<tr>
<th>energie</th>
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<th>hoofdquantum</th>
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<tr>
<td>eV</td>
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<td>getal n-</td>
<td>nm</td>
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<tr>
<td>0</td>
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<td>13,5950</td>
<td>∞</td>
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<td>13,0360</td>
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<td>4</td>
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<td>1</td>
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</tbody>
</table>

Fluorescent lamp

\[ hf = E_u - E_1 \]
Molecular energy levels

\[ hf = E_u - E_1 \]
Semiconductors

Valence band
Conduction band
Band gap

Molecular orbitals are plane waves
A $k$-vector points in the direction a wave is propagating.

Wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$

Momentum: $\vec{p} = \hbar \vec{k}$
Absorption and emission of photons

\[ hf = E_u - E_l \]

- Absorption
- Emission

Semiconductor

\[ hf < E_g \text{ no absorption} \]
What color light does a GaAs LED emit?

\[ E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda} \]

\[ \lambda = 867 \text{ nm} \quad \text{infrared} \]
Direct bandgap: \( \Delta k = 0 \)

Photons can be emitted.

Indirect bandgap: \( \Delta k \neq 0 \)

Phonons are emitted.

Momentum must be conserved when photons are absorbed or emitted.
Silicon band structure

$E_c = \text{bottom of the conduction band}$

$E_g = E_c - E_v$

$E_v = \text{top of the valence band}$

Electrons with energies in the gap are reflected out of the crystal.
### TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

<table>
<thead>
<tr>
<th>Material</th>
<th>Wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>InAsSbP/InAs</td>
<td>4200</td>
</tr>
<tr>
<td>InAs</td>
<td>3800</td>
</tr>
<tr>
<td>GaInAsP/GaSb</td>
<td>2000</td>
</tr>
<tr>
<td>GaSb</td>
<td>1800</td>
</tr>
<tr>
<td>Ga$<em>{1-x}$As$</em>{1-y}$P$_y$</td>
<td>1100-1600</td>
</tr>
<tr>
<td>Ga$<em>{0.47}$In$</em>{0.53}$As</td>
<td>1550</td>
</tr>
<tr>
<td>Ga$<em>{0.27}$In$</em>{0.73}$As$<em>{0.63}$P$</em>{0.37}$</td>
<td>1300</td>
</tr>
<tr>
<td>GaAs:Er,InP:Er</td>
<td>1540</td>
</tr>
<tr>
<td>Si:C</td>
<td>1300</td>
</tr>
<tr>
<td>GaAs:Yb,InP:Yb</td>
<td>1000</td>
</tr>
<tr>
<td>Al$<em>x$Ga$</em>{1-x}$As:Si</td>
<td>650-940</td>
</tr>
<tr>
<td>GaAs:Si</td>
<td>940</td>
</tr>
<tr>
<td>Al$<em>{0.11}$Ga$</em>{0.89}$As:Si</td>
<td>830</td>
</tr>
<tr>
<td>Al$<em>{0.4}$Ga$</em>{0.6}$As:Si</td>
<td>650</td>
</tr>
<tr>
<td>GaAs$<em>{0.6}$P$</em>{0.4}$</td>
<td>660</td>
</tr>
<tr>
<td>GaAs$<em>{0.4}$P$</em>{0.6}$</td>
<td>620</td>
</tr>
<tr>
<td>GaAs$<em>{0.15}$P$</em>{0.85}$</td>
<td>590</td>
</tr>
<tr>
<td>(Al$<em>x$Ga$</em>{1-x}$)$<em>{0.5}$In$</em>{0.5}$P</td>
<td>655</td>
</tr>
<tr>
<td>GaP</td>
<td>690</td>
</tr>
<tr>
<td>GaP:N</td>
<td>550-570</td>
</tr>
<tr>
<td>Ga$<em>{2}$In$</em>{1-x}$N</td>
<td>340, 430, 590</td>
</tr>
<tr>
<td>SiC</td>
<td>400-460</td>
</tr>
<tr>
<td>BN</td>
<td>260, 310, 490</td>
</tr>
</tbody>
</table>

**Light emitting diodes**

![Graph showing the relative eye response and emission wavelengths of light emitting diodes.](image)

- Infrared
- Red
- Green
- Violet
- Ultraviolet

- Orange Yellow

- $\lambda_m = 0.555 \mu m$

- FWHM

- $\lambda (\mu m)$
  - 1.0 0.8 0.7 0.6 0.5 0.45 0.4 0.35 1.2 1.6 2.0 2.4 2.8 3.2 3.6

- $E_g (eV)$
Metals, semiconductors, insulators

\[ E_g < 3 \text{eV} = \text{Semiconductor} \]
\[ E_g > 3 \text{eV} = \text{Insulator} \]

from: Singh
Copper dispersion relation and density of states

from Ibach & Lueth
Germanium

from Ibach & Lueth
Band gap

Electrons with energies in the gap are reflected out of the crystal.
Density of states

Silicon

Aluminum

\[ D(E) \]

Filled states

Empty states
Structural phase transition in Sn

$\alpha$-Sn, gray tin, diamond structure

$\beta$-Sn, white tin, tetragonal

$\alpha$-Sn transition at 13 C

金属 $\beta$ Sn
Structural phase transitions

Si, diamond structure

Si II, β-Sn, tetragonal

silicon makes a diamond to β-Sn transition under pressure
Fermi function

\[ f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \]

\( f(E) \) is the probability that a state at energy \( E \) is occupied.
Silicon density of states

$T = 300 \text{ K}$

$D(E) \ [\text{atom}^{-1} \text{eV}^{-1}]$

$\tilde{f}(E) D(E) \times 10^{12}$

$T = 300 \text{ K}$

electrons in the conduction band