The Physics of Infrared Detectors
(with a special emphasis on MID-IR detectors)

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Outline

• Semiconductors as crystals
• Energy bands
• Intrinsic semiconductors
• Light on intrinsic semiconductors
• Extrinsic Semiconductors
• Impurity band conductors (IBC)
**Periodic Table**

<table>
<thead>
<tr>
<th></th>
<th>IIB</th>
<th>IIIA</th>
<th>IVIA</th>
<th>VIA</th>
<th>VIA</th>
<th>VIIA</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹¹Al</td>
<td>Aluminium</td>
<td>³²Si</td>
<td>Silicon</td>
<td>³⁵P</td>
<td>Phosphorus</td>
<td>³⁴S</td>
</tr>
<tr>
<td>²⁶Ca</td>
<td>Copper</td>
<td>²⁴Zn</td>
<td>Zinc</td>
<td>²⁶Ga</td>
<td>Gallium</td>
<td>²⁴Ge</td>
</tr>
<tr>
<td>²⁴Ag</td>
<td>Silver</td>
<td>²⁴Cd</td>
<td>Cadmium</td>
<td>²⁴In</td>
<td>Indium</td>
<td>²⁴Sn</td>
</tr>
<tr>
<td>²⁴Au</td>
<td>Gold</td>
<td>²³Hg</td>
<td>Mercury</td>
<td>²³Tl</td>
<td>Thallium</td>
<td>³¹Pb</td>
</tr>
</tbody>
</table>

Atomic structure: (four $2s^2p$) covalent bonds per atom

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**Crystal Structure: 2-d**

- **Simple cubic**

Bravais lattice \( \vec{R} = m \vec{a} + n \vec{b} + p \vec{c} \)

In two dimensions, there are five distinct Bravais lattices

<table>
<thead>
<tr>
<th>Name</th>
<th>Number of Bravais lattices</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Square</td>
<td>1</td>
<td>( \vec{a}_1 = \vec{a}_2, \alpha = 90^\circ )</td>
</tr>
<tr>
<td>Rectangular</td>
<td>2</td>
<td>( \vec{a}_1 = \vec{a}_2, \alpha = 90^\circ )</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>1</td>
<td>( \vec{a}_1 = \vec{a}_2, \alpha = 120^\circ )</td>
</tr>
<tr>
<td>Oblique</td>
<td>1</td>
<td>( \vec{a}_1 = \vec{a}_2, \alpha = 120^\circ, \beta = 90^\circ )</td>
</tr>
</tbody>
</table>
Crystal Structure: 3-d

In three dimensions, there are fourteen distinct Bravais lattices

<table>
<thead>
<tr>
<th>Name</th>
<th>Number of Bravais lattices</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>1</td>
<td>$a_1 \neq a_2 \neq a_3, \alpha \neq \beta \neq \gamma$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>2</td>
<td>$a_1 = a_2 \neq a_3, \alpha = \beta = 90^\circ \neq \gamma$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>4</td>
<td>$a_1 \neq a_2 \neq a_3, \alpha = \beta = \gamma = 90^\circ$</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>2</td>
<td>$a_1 = a_2 \neq a_3, \alpha = \beta = \gamma = 90^\circ$</td>
</tr>
<tr>
<td>Cubic</td>
<td>3</td>
<td>$a_1 = a_2 = a_3, \alpha = \beta = \gamma = 90^\circ$</td>
</tr>
<tr>
<td>Trigonal</td>
<td>1</td>
<td>$a_1 = a_2 = a_3, \alpha = \beta = \gamma &lt; 120^\circ = 90^\circ$</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>1</td>
<td>$a_1 = a_2 = a_3, \alpha = \beta = 90^\circ, \gamma = 150^\circ$</td>
</tr>
</tbody>
</table>

A large number of semiconductors are cubic
($a_1 = a_2 = a_3 = a$ “lattice constant”)

Diamond Structure
Diamond Structure

Diamond Structure
Diamond Structure

Diamond Structure
Diamond Structure
Two interpenetrating face-centered cubic lattices

Diamond lattice: All same atoms (e.g. Si)

Zincblende lattice: different atoms in each sublattice (e.g. CdTe, GaAs)
Lattice planes in crystals: Miller indexes

Silicon and Germanium break on \{1,1,1\} planes

*never confuse the spacing between lattice planes with the spacing between crystal planes*

Example

The surface density of Silicon is

\[
\begin{align*}
11.8 \times 10^{14} \text{ atoms/cm}^2 & \text{ on } \{111\} \\
9.6 \times 10^{14} \text{ atoms/cm}^2 & \text{ on } \{110\} \\
6.8 \times 10^{14} \text{ atoms/cm}^2 & \text{ on } \{100\}
\end{align*}
\]
The smallest ("primitive") cell which displays the full symmetry of the lattice is the Wigner-Seitz cell.

Construction method: surfaces passing through the middle points to the nearest lattice points. In 3-d think to a polyhedron.

Wigner-Seitz cell construction
Reciprocal lattice

\[ \bar{\mathbf{g}} = h\bar{a} + k\bar{b} + l\bar{c} \]

The Bravais lattice after Fourier transform

<table>
<thead>
<tr>
<th>real space</th>
<th>reciprocal lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>normals to the planes (vectors)</td>
<td>points</td>
</tr>
<tr>
<td>spacing between planes</td>
<td>1/distance between points</td>
</tr>
<tr>
<td>(\lambda) (distance, wavelength)</td>
<td>2(\pi/\lambda)=(k) (momentum, wave</td>
</tr>
<tr>
<td></td>
<td>number)</td>
</tr>
<tr>
<td></td>
<td>(actually, (2\pi/distance))</td>
</tr>
</tbody>
</table>
Bragg conditions

When a wave impinges on a crystal - and it doesn't matter if it is an electromagnetic wave, e.g. X-rays, or an electron, or neutron "wave" - it will be reflected at a particular set of lattice planes \([hkl]\) characterized by its reciprocal lattice vector \(\mathbf{g}\) only if the so-called **Bragg condition** is met

\[
\mathbf{k} - \mathbf{k}' = \mathbf{g}
\]

If the Bragg condition is *not* met, the incoming wave just moves through the lattice and emerges on the other side of the crystal (neglecting absorption)

Elastic scattering

\[
|\mathbf{k}| = |\mathbf{k}'|
\]

For a given \(k\), The Bragg conditions is met on surfaces normal to particular \(g\).
These surfaces define cells in the \(k\)-space, called **Brillouin zones**
Brillouin Zone construction

All wave vectors that end on a BZ, will fulfill the Bragg condition and thus are diffracted. Wave vectors completely in the interior of the 1. BZ, or in between any two BZs, will never get diffracted; they move pretty much as if the potential would be constant, i.e. they behave very close to the solutions of the free electron gas.

Brillouin zone

The Brillouin zone is defined in the reciprocal lattice.

The first BZ is the volume enclosed within a Wigner-Seitz cell in the k-space.

In 3-d think to a nested set of polyhedra
# WS zone and BZ

<table>
<thead>
<tr>
<th></th>
<th>Lattice Real Space</th>
<th>Lattice K-space</th>
</tr>
</thead>
<tbody>
<tr>
<td>bcc WS cell</td>
<td><img src="image" alt="bcc WS cell" /></td>
<td>Bcc BZ (fcc lattice in K-space)</td>
</tr>
<tr>
<td>fcc WS cell</td>
<td><img src="image" alt="fcc WS cell" /></td>
<td>fcc BZ (bcc lattice in K-space)</td>
</tr>
</tbody>
</table>

The WS cell of bcc lattice in real space transforms to a Brillouin zone in a fcc lattice in reciprocal space while the WS cell of a fcc lattice transforms to a Brillouin zone of a bcc lattice in reciprocal space.

Bcc: body-centered cubic; fcc: face-centered cubic

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# Brillouin zone of Silicon

Points of high-symmetry on the Brillouin zone have specific importance. The most important point for optoelectronic devices is the center at $\mathbf{k} = \mathbf{0}$, known as the gamma point $\Gamma$.

Note the points $\Gamma$, $X$, $W$, $K$, …
Wave vectors near or at a BZ - let's call them $k_{\text{BZ}}$ electrons - feel the periodic potential of the crystal while the others do not. E.g., they are diffracted.

**ENERGY GAP in CRYSTALS**

- On the BZ it is $k=-k$: these are two standing waves described by $\psi \sim e^{ikr}$ and $\psi \sim e^{-ikr}$
- Their combination can be symmetric
  $$\psi_+ \sim e^{ikr} + e^{-ikr} \sim \cos(kr)$$
  or antisymmetric
  $$\psi_- \sim e^{ikr} - e^{-ikr} \sim \sin(kr)$$
- The probability density $\psi^* \psi$ have different values at each point
- 2 different values of the energy, varying with $k$ on the BZ: ENERGY GAP.
Two energy values at $k = k_{BZ}$

$$E(k_{BZ}) = \frac{(\hbar k)^2}{2m} \pm U(g)$$

Energy bands

F. Block solved the Shroedinger equation for an electron in the lattice:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi_k(r) = E_k \psi_k(r)$$

If $V(r)$ is periodic with periodicity of the lattice, then the wave function is a plane wave (free electron) with periodic modulation

$$\psi_k(r) = e^{ik \cdot r} U_n(k, r) = \text{Block function}$$

$k$ is a wave vector in the reciprocal lattice, $U_n(k, r)$ is periodic in $r$, i.e. $U(r+R) = U(r)$, and $n$ is the band index.

- For a given $n$, it is sufficient to use $k$’s in the primitive cell of the reciprocal lattice (Brillouin zone). The rest is redundant!
Band Structure and Bloch’s Theorem

From:

\[ \psi_k(r) = e^{i k \cdot r} U_n(k, r) = \text{Block function} \]

It is also:

\[ \psi_{k+g}(r) = e^{i (K+g) \cdot r} U_n(k+g, r) = \psi_k(r) \]

Then:

\[ E(k+g) = E(k) \]

for dispersion curves that have a different origin

There are many energy values for one given \( k \). In particular, all possible energy values are contained within the first Brillouin zone (between -1/2\( g_1 \) and +1/2\( g_1 \) in the picture).

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Band Structure and Bloch’s Theorem

reduced representation of the band diagram

Every energy branch in principle should carry an index denoting the band (often omitted)

Energy functions of a periodic potential

The electron at \( k \) can go to the upper band if someone gives him

1. \( \Delta E > \text{bandgap} \), AND
2. \( k_f = k_i + g \)

(BRAGG LAW FOR INELASTIC SCATTERING)
Band diagram of Silicon

- Si has a band gap of about 1 eV.
- Si is an indirect semiconductor because the maximum of the valence band (at Γ) does not coincide with the minimum of the conduction band (to the left of X).

Direct and Indirect Semiconductors

- Generation: \( \Delta E = h\nu \)
- Recomb. not allowed
Astronomer’s band diagram

\[ \lambda_{co} = \frac{1.24}{E_g (eV)} \]

Conduction band

Valence band

\[ E_g \text{ bandgap} \]

Fermi Energy and Carrier Concentration

The number (or density) of something is given by the density of available places times the probability of occupation.

Density of electrons in the energy interval \( E, E + \Delta E = \)
density of states \( \times \) probability for occupancy \( \times \) energy interval

\[ dN = D(E) \cdot f(E, T) \cdot dE \]
Density of states

A free (or under constant potential) particle in a rectangular box has:

1) only kinetic energy
\[ E_k = \frac{\hbar^2 k^2}{2m} \]

2) \( k \) is discrete (stationary waves)
\[ k_{x,y,z} = \pm \frac{2\pi}{L} n_{x,y,z} \]

Therefore, the energy is quantized
\[ E_n = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 \left( n_x^2 + n_y^2 + n_z^2 \right) \]

Density of states \( D_s \)

- In phase space a surface of constant energy is a sphere.
  The volume is
  \[ V = \frac{4}{3} \pi k^3 \]
- Any "state", i.e. solution of the Schrödinger equation with a specific \( k \), occupies with 2 electrons the volume
  \[ V_s = \left( \frac{2\pi}{L} \right)^3 \]
- The number of cubes fitting inside the sphere at energy \( E \) thus is the number of all energy levels up to \( E \):
  \[ N_s = 2 \frac{V}{V_s} = \frac{k^3 L^3}{3 \pi^2} \]

Finally:
\[ D_s = \frac{1}{L^3} \frac{dN_s}{dE} = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \]
Density of states $D_s$

At 0 K one can place electrons up to the Fermi level $E_F$

Probability of occupancy

Fermi distribution

$$f(E, T) = \frac{1}{e^{\frac{E - E_F}{kT}} + 1}$$
Intrinsic Semiconductors

The concentration of electrons in the conduction band is

\[ n^e = \int_{E_g}^{\infty} D(E) f(E, T) dE \]

\[ \approx N_e^{\text{eff}} e^{\frac{E - E_g}{kT}} \]

\[ \approx A T^{3/2} e^{-\frac{E_g}{2kT}} \]

The number of electrons in the conduction band depends on \( E_g \) and \( T \).

In Si \( n^e \) doubles for \(~8\) degree rise in temperature.
Same for the holes in the valence band:
\[ n_e = n_h = n_i \quad \text{“INTRINSIC CONCENTRATION”} \]

Mass action law:
\[ n^2 = n_e n_p = 4 \left( \frac{2\pi kT}{\hbar^2} \right)^3 e^{-\frac{E_g}{kT}} \left( m_e^* m_h^* \right)^{3/2} \]

The bandgap energy and the effective mass depend on T for Silicon:
\[ E_g(300 \text{ K}) = 1.1242 \text{ eV} \]
\[ E_g(0 \text{ K}) = 1.700 \text{ eV} \]

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**Conductivity**

The CONDUCTIVITY
\[ \sigma = e \left( \mu_e n_e + \mu_h n_h \right) \]

decreases with \( E_g \). Leakage currents are lower in large \( E_g \) materials.

The mobility \( \mu \) is the proportionality constant between the average drift velocity \( v_D \) of carriers in the presence of an electrical field \( E \):
\[ v_D = \mu E \]

Mobility depends on the average time between scattering processes
\[ \mu = \frac{\sigma}{m} \]
Radiation on intrinsic semiconductors

- at low T the conduction band is “empty”. Low intrinsic conductivity
- radiation with $h\nu > E_g$ creates electron-hole pairs: $n^e = n^h$
- both electrons and holes contribute to the photocurrent, depending on mobilities
- The conductivity changes: PHOTOCONDUCTOR
  \[ \sigma = e \left( \mu^e n^e + \mu^h n^h + \mu^e \Delta n^e + \mu^h \Delta n^h \right) \]
  Where
  \[ \Delta n^{e,h} = \eta \text{ (quantum efficiency)} \times \Phi \text{ (photon flux)} \]
  (neglecting recombination time, etc)
- all atoms count: absorption occurs in thin layer (~10micron)

Extrinsic semiconductors

Extrinsic semiconductors are formed by adding acceptor and donor atoms to the intrinsic semiconductor. This changes the electronic properties, allowing for increased conductivity and sensitivity to radiation.
The ruby mineral (corundum) is aluminum oxide with a small amount (about 0.05%) of chromium which gives it its characteristic pink or red color by absorbing green and blue light.
Charge neutrality \( n^e + N_A^- = n^h + N_D^+ \) gives \( E_F \) and therefore the concentrations

**Extrinsic semiconductors**

Normally \( N_D \neq N_A \)

“Dopant or majority” vs. “residual impurities”

Ex: Si:Ga (III group) is p-type \( N_D \leq N_A \)
Si:As (V group) is n-type \( N_D \geq N_A \)

- There are shallow- and deep-level impurities
- shallow-level impurities increase the \( \lambda \) response
- Atoms of dopant and residual impurities do not interact with each other.

Example p-type: at low \( T \) the conduction band is “empty”; donor impurities have lost their electrons and are ionized, acceptor dopant has electrons from valence band and impurities; valence band has free holes.
Opposite requirements

To move away and collect charges we need an electric field:

\[ E_x = \frac{dV}{dx} \]

To have a good drop of potential, no current must flow:
Detector material must have high impedance
(I.e. low conductivity)

On the other hand, we want high concentration of absorbers:
this goes in the direction of high conductivity

Impurity band conduction

The donor band (As in Si:As) can be heavily doped
Photons are absorbed
• in thin layer (smaller volume)
• providing higher QE
• higher radiation immunity
• lower applied bias
• better uniformity
• faster response

High dopant concentration creates a band ~1meV wide, thus the cutoff increases from 24 to 28µm.
However:

The donor band becomes a conduction band:
“Impurity Band Conduction”
Impurity band conduction

The donor band (As in Si:As) is heavily doped.
Electric field is applied (bias) and the free charge carriers are driven out from the IR active region (depletion):
High resistance and high electric field

Problem: charges “hop” in the impurity conduction band;
If they are sensed there is an extra dark current: need for a blocking layer (BIB)

Photo-electrons and relative holes are collected
Si:As Engineering

- Dopant As is n-type. P-type impurities (e.g. B) are a potential problem
- They are “neutralized” by As, leaving them as negative charge centers in the “depletion region”
- These \( N_A \) charges create an electric field that limits the extension of the depletion region \( w \)

Poisson equation for the ionized impurities:

\[
\frac{dE}{dx} = \frac{\rho}{\varepsilon_0} = \frac{-eN_A}{\varepsilon_0} = \frac{k_B T}{\varepsilon_0}
\]

The width of the depletion region depends on the bias and on the impurity concentration

Assuming \( N_A = 10^{12} \text{ cm}^{-3} \) and \( V_b = 1 \text{V} \) it is \( w = 32 \mu\text{m} \)
An acceptable arsenic concentration is \( N_D = 3 \times 10^{17} \text{ cm}^{-3} \).
For arsenic in silicon, the absorption cross section is \( \alpha_{\text{Si:As}} = 2.2 \times 10^{-15} \text{ cm}^2 \)
the absorption length is \( l = l/N_D \alpha_{\text{Si:As}} = 15 \mu\text{m} \).

Since \( l \ll w \), a high quantum efficiency detector can be built.

Most of the failures in detector processing have to do with unwanted impurities, and the improvement of the performance of this detector type is closely linked to driving down \( N_A \).

Spitzer Si:As (BIB) 128x128 array