Material Properties of Silicon

- Band structure and Optical absorption
- Doping
- Recombination
- Carrier Transport
1. Optical Properties of Silicon

Indirect Band-gap

Phonon is needed – reduces absorption

Refractive index = 3.4; reflectivity = 40 % for visible light. Can be reduced by AR coating.
2. Doping by Impurities

- Silicon crystal in pure form is good insulator - all electrons are bonded to silicon atom

- Replacement of Si atoms can alter electrical properties of semiconductor

- Group number - indicates number of electrons in valence level (Si - Group IV)

<table>
<thead>
<tr>
<th>IIIB</th>
<th>IVB</th>
<th>VB</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>C</td>
<td>N</td>
</tr>
<tr>
<td>Boron</td>
<td>Carbon</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>2-3</td>
<td>2-4</td>
<td>2-4</td>
</tr>
<tr>
<td>Al</td>
<td>Si</td>
<td>P</td>
</tr>
<tr>
<td>Aluminum</td>
<td>Silicon</td>
<td>Phosphorous</td>
</tr>
<tr>
<td>2-4-3</td>
<td>2-4-4</td>
<td>2-4-6</td>
</tr>
<tr>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
</tr>
<tr>
<td>Gallium</td>
<td>Germanium</td>
<td>Arsenic</td>
</tr>
<tr>
<td>2-4-10-3</td>
<td>2-4-10-4</td>
<td>2-4-10-6</td>
</tr>
</tbody>
</table>
Doping-induced changes in energy levels

- Energetically, doping introduction of a permitted energy level in the forbidden gap.

### p-type doping

- $E_C$ (Conduction Band)
- $E_V$ (Valence Band)

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Band Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T = 0 , \text{K}$</td>
<td><img src="image1.png" alt="Diagram" /></td>
</tr>
<tr>
<td>$T$</td>
<td><img src="image2.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>

### n-type doping

- $E_C$ (Conduction Band)
- $E_V$ (Valence Band)

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Band Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T = 0 , \text{K}$</td>
<td><img src="image3.png" alt="Diagram" /></td>
</tr>
<tr>
<td>$T$</td>
<td><img src="image4.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>

Room $T$
p and n-type semiconductors

Intrinsic semiconductor - Si

n-type semiconductor – SiP

- Additional (donor) levels appear at CB
- Dominant carriers → electrons; n-type
Recombination Processes

(i) Radiative

(ii) Auger

(iii) Trap-assisted Recombination
Recombination Processes

Diagram showing band-to-band, trap-assisted, and Auger recombination processes.
Recombination Processes in Si

- **Radiative recombination** rate in p-type \( U_{rad} = \frac{n - n_0}{\tau_{n,rad}} \)

  Radiative lifetime varies as \( 1/N_a \).
  For p-type Si, it is of the order of milliseconds. So \( U_{rad} \) is negligible.
  Never dominant in practical solar cells.
  \((n, n_0 \) are number of electrons under bias and equilibrium, respectively\)

- **Auger recombination** in Si is important at high doping density (~ \( 10^{17} \) cm\(^{-3} \)) and high temperatures.
Recombination Processes in Si

- **Shockley-Read-Hall** (SRH) recombination = Trap assisted recombination

\[ U_{SRH} = \frac{n - n_0}{\tau_{n,SRH}} \]

\( \tau_{n,SRH} \) the minority carrier lifetime depends on density of trap states and their position in the band-gap.

In lightly doped p-type Si, \( \tau \sim 10 \ \mu \text{sec.} \)

In lightly-doped n-type Si, it is \( \sim 1 \ \mu \text{sec.} \)
Surface Recombination in Si

- Surface recombination is important when minority carrier diffusion lengths are long.

- Surface recombination velocity $= 10^3 – 10^5 \text{ cm.s}^{-1}$ for untreated surfaces and at interfaces with metallic contacts.

- When surface is passivated with a layer of silicon dioxide, the recombination velocity reduces $< 100 \text{ cm.s}^{-1}$ because oxide layer shields minority carriers from defects.
Carrier Transport

- Electron mobility in p-type Si is more than hole mobility in n-type Si.

- Carrier collection is more efficient in p-type than n-type because fundamental impurities are acceptor type.

- Electron and hole mobilities are determined by frequency of scattering events.

<table>
<thead>
<tr>
<th>Si</th>
<th>Electrons cm²V⁻¹s⁻¹</th>
<th>Holes cm²V⁻¹s⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mobility (low doping)</td>
<td>1500</td>
<td>500</td>
</tr>
<tr>
<td>Mobility (high doping)</td>
<td>70</td>
<td>50</td>
</tr>
</tbody>
</table>

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General features of p-n junction

- Thickness should be more than absorption length
- Junction should be shallow compared to diffusion length to avoid dead layer
- Emitter should be doped heavily – improves conductivity with metallic contacts
- Reflection should be minimized – Anti-reflection coatings are used
Basic structure of Si solar cell

A typical Si solar cell is n-p junction made in a wafer of p-type Si.

<table>
<thead>
<tr>
<th>Anti-reflection coating</th>
<th>Front contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emitter</td>
<td>n-type (heavily doped ( \sim 10^{19} \text{ cm}^{-3} ))</td>
</tr>
<tr>
<td>Base</td>
<td>p-type (lightly doped ( \sim 10^{16} \text{ cm}^{-3} ))</td>
</tr>
<tr>
<td>Rear contact</td>
<td></td>
</tr>
</tbody>
</table>

0.3 \( \mu \text{m} \)

300-500 \( \mu \text{m} \);
Area = 100 cm\(^2\)
Si solar cell fabrication

- Single crystal Si wafer is grown by Czochralski or Float zone process
- Boron is introduced during growth to produce $p$-type crystal
- Junction is prepared by diffusing $n$-type dopant (usually P) on the $p$-type wafer.
- P is deposited either from vapour phase or by exposure to N+POCl$_3$ gas.
**Steps of Fabrication**

- First step is refining silicon.
- Silicon dioxide ($\text{SiO}_2$) is the most abundant mineral in the earth's crust.
- The manufacture of the hyper pure silicon for photovoltaics starts with locating a source of silicon dioxide in the form of sand.
- The silica is reduced (oxygen removed) through a reaction with carbon in the form of coal, charcoal and heating to 1500-2000 °C in an electrode arc furnace.
Steps of Fabrication

- Silicon dioxide + Carbon = Silicon + Carbon dioxide

- The resulting silicon is 98% pure. It contains Fe, Al, and B, to remove these traces, further purification is done,
  Powdered Si is reacted with anhydrous HCl at 300 °C to form SiHCl₃

\[
\text{Si} + 3\text{HCl} \Rightarrow \text{SiHCl}_3 + \text{H}_2
\]
Variation of energy levels inside a cell

Junction is diffused – so electric field is extended from the surface
Front surface is textured to reduce reflectivity

- Refractive index of AR coating = 2 and thickness is 80-100 nm.
- Suitable materials for AR coating are: Ta$_2$O$_5$, TiO$_2$ and Si$_3$Ni$_4$
- Back surface is heavily doped to reduce surface recombination
Optimization of Si cell design

- Absorption of light close to the band gap (near infrared) is poor
- Bulk recombination in the $p$ region is the most important one
- Rear surface recombination is important, particularly for photogeneration by red and infrared light
The challenges are to:

- Maximize absorption
- Minimize rear surface recombination
- Minimize series resistance
1. To enhance absorption: Texturing

Front surface is textured either by chemical treatment or photolithography.
Optimization of contacts:

- Shading the front surface by metal contact reduces area available for light absorption by 10%.

- So contact area can be reduced by making “buried contacts”

- Grooves can be created by laser or mechanical etching
BURIED CONTACT FABRICATION TECHNOLOGY

- Textured front with SiO₂ passivation
- Light emitter diffusion
- Copper plating in laser cut grooves
- Heavy phosphorous diffusion in grooves
- P-type substrate
- Aluminium alloyed BSF
- Rear copper contact
2. To reduce surface recombination

- Passivation of front surface with thin oxide coating
- Using point contacts at the rear
- Si-Metal interface is more defective than Si-SiO₂ interface
3. To reduce series resistance:


2. Differential doping around the contact area – by exposing the contact areas to dopant-rich gases before deposition of the contacts.

3. Formation of narrow but deep finger contacts – surface area blocked by contacts is reduced; high contact area between fingers and semiconductor reduces current density at the contact.