Classes of Photovoltaic Materials

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Efficiency vs. Theoretical Max.

Efficiency: % of incident radiation power available for electrical work

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>CPV (3J)</td>
<td>63%</td>
<td>31%</td>
<td>43.5%</td>
</tr>
<tr>
<td>c-Si</td>
<td>29%</td>
<td>18%</td>
<td>27.6%</td>
</tr>
<tr>
<td>mc-Si &quot;poly&quot;</td>
<td>29%</td>
<td>20.4%</td>
<td>15%</td>
</tr>
<tr>
<td>CIGS</td>
<td>29%</td>
<td>20.3%</td>
<td>13%</td>
</tr>
<tr>
<td>CdTe</td>
<td>29%</td>
<td>17.3%</td>
<td>12%</td>
</tr>
<tr>
<td>a-Si</td>
<td>20%</td>
<td>12.5%</td>
<td>10%</td>
</tr>
<tr>
<td>OPV</td>
<td>14%</td>
<td>8.3%</td>
<td>2%</td>
</tr>
</tbody>
</table>

Source: NREL

Theoretical max. → typical assumptions
- Perfect absorption above energy gap
- One photon = one e-h pair
- No non-radiative losses
- Lossless transport of charges
- Thermal eqm @ T=300K

Approaching theoretical max. is a scientific & engineering research challenge
Despite moderate efficiency and high life-cycle costs, crystalline Si cells retain >80% market share.
Efficiency is key, but it's not everything

- Global power consumption ~20 TW
  - Peak daily average solar insolation ~ 300 W/m²
  - Solar replace consumption ⇒ 670,000 km² @ 10% efficiency
  - Grid parity ⇒ ~cover area of Texas!
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• Economics is critically important!
  – Abundance of constituents
  – Cost of production and deployment
  – Life-cycle management of materials

• But: efficiency is a strong economic factor
  – Affected by materials class (theoretical max.)
  – Engineering (control loss & approach theoretical max.)
  – Ample research opportunities from materials science to device engineering
Outline

• **Inorganics**
  - Silicon: crystalline, poly-crystalline
  - Thin films: GaAs, InP, CdTe, CIGS; tandems, amorphous Si
  - Bulk Pvs, perovskites

• **Inorganic/organic hybrids**
  - Dye-sensitized cells

• **Organics**
  - BHJ cells, donors and acceptors
  - Electrodes and TCOs
  - Evaporated small-molecule cells
Mono-crystalline Si cells

Mature technology
Earth-abundant low-cost constituents
Leverage microelectronics industry
Easy to dope
Charge separation by p-n junction (no losses to interface states)
High efficiency (record 27%, theoretical max. 29%)

Expensive and energy intensive fab.
Thick material (low optical absorption strength)
~200-300 μm
Requires quality crystal for long-range carrier diffusion
Quite reflective (without optical coatings or texturing)

Diamond, space group Fd3m

Image source: wikipedia.org
Poly-crystalline Si

Less costly and energy intensive c.f. single crystal

Squared edges – better cell packing in module

Lower efficiency
- carrier loss at grain boundaries
Alternative single-crystal materials

Zinc blende, space group $F\bar{4}3m$

Compound semiconductors: GaAs, AlGaAs, InP, GaSb

- Direct-gap strong optical absorption
- Thinner devices, $\sim 5 \, \mu m$
- More efficient carrier extraction
- Tolerate lower crystal quality
- Low weight (space applications)
- Radiation hardness (space applications)
- Dopants available for p-n junctions
- Better carrier mobilities
- Tandem cells possible (higher efficiency)

~5x more expensive than Si

Not terrestrially abundant:
Unlikely to scale to TW
Suitable substrates - expensive

Image: JPL/NASA

Thin-film Photovoltaics: CIS/CIGS

Ternary semiconductors: CuInSe2, Cu(In:Ga)Se2

Even stronger absorption than GaAs
Direct gap (~1 eV)
Thinner films (2-4 μm)
Flexible
Tolerate shorter diffusion length
Alloy with Ga to optimize (increase) gap

Dopants:
- p-type is natural (native defects, In vacancy)
- n-type is difficult
Best: heterojunctions with CdS emitter
21% record efficiency

Indium & gallium are not abundant
Heterostructure: trap states at grain boundaries
Interface forms small Schottky barrier
- Photocharges must tunnel
Diffusion of species across interface, polymorphs

Global Solar's 750kW CIGS array

www.globalsolar.com
Other thin film technologies

• Amorphous Si
  – Tetrahedrally coordinated with no LR order
    • Relaxed optical selection rules
    • Direct band gap, very strong absorption
  – Poor doping quality
    • carriers trapped at dangling bonds
    • Passivation with H improves, but increases gap beyond optimal
  – Poor carrier diffusion length, especially in doped material
  – p-i-n junction design with blanket TCO electrode

• CdTe
  – Heterostructure with n-CdS
  – Efficient, flexible
  – No tunnel barrier (c.f. CIGS), but lattice mismatch
  – Te is really rare
  – Record efficiency 19.6%

Greenough River Solar Farm
150,000 CdTe panels
Inorganic Perovskite Photovoltaics

Ferroelectric perovskite oxides
- Switchable electric polarization in crystal
- Bulk driving force for charge separation
- Interface or p-n junction not required
- Photocurrent direction switch with P
- Highly experimental

\[
[K\text{NbO}_3]_1 - x[B\text{aNi}_{1/2}\text{Nb}_{1/2}\text{O}_3 - \delta]_x (\text{KBNNO})
\]

Grinberg et al., Nature 503, 509 (2013)

\[\sim 10 \text{ nA at } 3.5 \text{ V} \Rightarrow 0.04 \mu\text{W/W}\]
Terrestrial Abundance of Elements

Abundance, atoms of element per $10^6$ atoms of Si

0  10  20  30  40  50  60  70  80  90

Atomic number, Z

10^{-6}  10^{-3}  10^0  10^3  10^6  10^9

Rock-forming elements

Major industrial metals in red
Precious metals in purple
Rare earth elements in blue
Rarest "metals"