Why PS?
Outline

- History
- Overview of PS
- Synthesis:
  - Mechanisms
  - Steps
  - Tacticity
- Some reaction to polystyrene
- Properties
  - Physical
  - Thermal
  - Mechanical
- Polystyrene Products
- Polystyrene Recycling
- Conclusion
Polystyrene (PS), like most polymers, was accidentally discovered in Berlin in 1839 by a pharmacist named Eduard Simon.
Overview

- **Monomer(s):** Styrene (reaction below)
- **Contains:** Phenyl rings
- **Mn Range:** 100,000–400,000
- **Key Characteristic:** Thermoplastic
Synthesis

- **Mechanism:**
  Addition

- **This includes:**
  free radicals, cationic, anionic

- **Steps:**
  Initiation, Propagation, Termination
Synthesis Steps

- **Initiation:**
  
  1. \[ \text{H-O-O-H} \xrightarrow{\text{heat}} 2\text{H-O}^* \]
     
     \[
     \begin{array}{c}
     \text{hydrogen peroxide} \\
     \text{free radicals}
     \end{array}
     \]

     \[
     \begin{array}{c}
     \text{H-O}^* + \text{C}=\text{C} \rightarrow \text{H-O-C-C}^* \\
     \text{free radical} \\
     \end{array}
     \]

     \[
     \begin{array}{c}
     \text{styrene} \\
     \end{array}
     \]

- **Propagation:**
  
  \[
  \begin{array}{c}
  \text{H-O-C-C}^* + \text{C}=\text{C} \rightarrow \text{H-O-C-C-C-C}^* \\
  \end{array}
  \]
Synthesis Steps

- **Termination:**
  1. Combination

\[
\text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_n \cdot \text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_m \rightarrow \text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_n \begin{array}{c|c|c} \text{C} & \text{C} \end{array}_m \text{CO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_m
\]

2. Disproportionation

\[
\text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_n \cdot \text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_m \rightarrow \text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_n \begin{array}{c|c|c} \text{C} & \text{H} \end{array}_m + \text{HO-} \begin{array}{c|c|c} \text{H} & \text{H} \end{array}_n \begin{array}{c|c|c} \text{C} & \text{C} \end{array}_m
\]
Tacticity and Crystallinity

Commercial
Mostly amorphous

Isotactic  Syndiotactic  Atactic

Increase crystallinity
Commercial
\[ \text{CCl}_3 + \text{CH}_2\text{=CH}_2 \rightarrow \text{Cl}_3\text{CCH}_2\cdot\text{CH}_3 \rightarrow \text{Cl}_3\text{CCH}_2\text{C}_6\text{H}_5 \]

Styrene

\[ \text{Cl}_3\text{CCH}_2\text{C}_6\text{H}_5 \rightarrow \text{etc.} \]

\[ \text{Cl}_3\text{C} - \text{CH}_2 - \text{C} - \text{C} - \text{C} - \text{C}_6\text{H}_5 \]
Scheme II:

\[ \text{Styrene} \quad \text{TsOMI} \quad \text{AIBN} \quad 60-90^\circ \text{C.} \]

Poly(styrene-co-[N-(tosyloxy)maleimide])
# Forms of PS

<table>
<thead>
<tr>
<th>General Purpose PS (GPPS)</th>
<th>High Impact PS (HIPS)</th>
<th>Expanded PS (EPS)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Image of General Purpose PS" /></td>
<td><img src="image2" alt="Image of High Impact PS" /></td>
<td><img src="image3" alt="Image of Expanded PS" /></td>
</tr>
</tbody>
</table>
## Forms of PS

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</thead>
<tbody>
<tr>
<td><strong>Characteristics</strong></td>
<td>Clear, hard, brittle</td>
<td>Tough, hard</td>
<td>Tough, lightweight, rigid-foam</td>
</tr>
<tr>
<td><strong>Cost index ($/lbs)</strong></td>
<td></td>
<td>≤ 0.9</td>
<td></td>
</tr>
<tr>
<td><strong>Embodied energy (MJ/kg)</strong></td>
<td>86.40</td>
<td>87.40</td>
<td>88.60</td>
</tr>
<tr>
<td><strong>Trade names</strong></td>
<td>Dylene (Arco)</td>
<td>Bextrene</td>
<td>Styropor (BASF), Styrofoam</td>
</tr>
</tbody>
</table>
# Physical Properties

<table>
<thead>
<tr>
<th></th>
<th>General Purpose PS (GPPS)</th>
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<th>Rubber bands (natural)</th>
<th>Legos (ABS)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Density (g/cm³)</strong></td>
<td>1.05</td>
<td>1.04</td>
<td>0.008-1.10</td>
<td>0.9-1.0</td>
<td>1.06</td>
</tr>
<tr>
<td><strong>Glass Transition T (°C)</strong></td>
<td>100</td>
<td>100</td>
<td>-70</td>
<td>100</td>
<td></td>
</tr>
</tbody>
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## Thermal Properties

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</thead>
<tbody>
<tr>
<td><strong>Thermal Conductivity</strong></td>
<td>0.14</td>
<td>0.22</td>
<td>0.027-0.0418</td>
<td>0.14</td>
<td>0.23</td>
</tr>
<tr>
<td><strong>(W/m-K)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Thermal Expansion</strong></td>
<td>120</td>
<td>80</td>
<td>0.08-70</td>
<td>225</td>
<td>95</td>
</tr>
<tr>
<td><strong>(µm/m-K) (20°C)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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### Mechanical Properties

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</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus (GPa)</td>
<td>2.9</td>
<td>1.9</td>
<td>0.0065-0.04</td>
<td>-</td>
<td>1.9</td>
</tr>
<tr>
<td>UTS (MPa)</td>
<td>46</td>
<td>80</td>
<td>0.08-0.911</td>
<td>3.5-35</td>
<td>40</td>
</tr>
<tr>
<td>Elongation at break (%)</td>
<td>2%</td>
<td>40%</td>
<td>5-13.4%</td>
<td>300-900 %</td>
<td>20%</td>
</tr>
</tbody>
</table>
Polystyrene Products

- Sheet or Molded
- Disposable Cutlery
- CD
- Foams
- Insulation (Thermal & Acoustic)
- Packaging
- Shock Absorption
Lab supplies (GPPS)

Packaging (EPS)

Food containers (HIPS)
Polystyrene Recycling

Polystyrene can not be recycled

Polystyrene Disposal:
- Burial (Landfill)
  Stable to bury (without contamination)
  Without UV and oxygen long degradation times
- Incineration
  Requires high temperatures to combust properly
  High energy content (good fuel)
- Discarded (Thrown away into the environment)
- Reduce / Reuse / Recycle
**Conclusion**

- **Polystyrene (PS)** is a thermoplastic polymerized from styrene monomer by addition.
- **Cheap to produce**, hence one of the most popular polymers.
- **Pure PS** is brittle (GPPS), adding polybutadiene makes it tougher (HIPS).
- **Foam form of PS** can be produced by adding a blowing agent (EPS).
- **Applications** include packaging and containers.