Heterojunction Based Hybrid Si Nanowire Solar Cell

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Material Growth
Surface Engineering
Characterization
Devices prototype
Table of Contents

Introduction
Important Features of Nanowires
Obstacles
Molecules

First Chapter: Growth of Silicon Nanowire
Top Down

Second Chapter: Surface Treatment & Characterization
Termination with Molecules: Grignard Reaction
Surface Transfer Doping

Third Chapter: Devices
Solar Cell

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Introduction

Important features of Nanowires
Obstacles
Molecules
Important features of Nanowires

- They represent the smallest efficient transport
- Increased surface scattering
- Orthogonal Junction
- Increased surface area
- Integration & Devices

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Obstacles for nanowire growth and surface modifications:

Native oxides

SiO$_2$ → Si

Lowest surface densities ever reported with thermal oxides! $\sim 10^{10}$ cm$^{-2}$ (Si surface density $\sim 10^{14}$ cm$^{-2}$). However:

**Amorphous oxides:**
(i) Dangling bonds
(ii) Induces trap states at the SiO$_2$/Si interface
(iii) Limits the effect of gate voltage
(iv) No direct chemistry with Si


Gold diffusion

Gold can behave as a catalyst. However:
(i) has a high diffusion coefficient $10^{-6}$ cm$^{-2}$sec ($10^{-9}$-$10^{-14}$) at 1100°C
(ii) Induces deep states inside the band gap

Obstacles on the Road

Obstacles for nanowire growth and surface modifications:

Native oxides

Gold diffusion

Lowest surface densities ever reported with thermal oxides! $\sim 10^{10}$ cm$^{-2}$ (Si surface density $\sim 10^{14}$ cm$^{-2}$). However:

Amorphous oxides: (i) Dangling bonds

(ii) Induces trap states at the SiO$_2$/Si interface

(iii) Limits the effect of gate voltage

(iv) No direct chemistry with Si

A promising approach to overcome the aforementioned obstacles is to use molecules. Main advantages are as follows:

- Terminating dangling bonds → low surface state density
- Systematic dipoles → (work function design, surface dipoles)
- Negative dipoles
- Positive dipoles
- Controlling the molecular density
- Controlling cross-linking
- Stabilizing the surface (superior oxidation resistance)
- Molecular surface transfer doping: Controlling the doping level and type (p or n) through organic molecules.
Chapter 1
Realizing \textbf{Si Nanowires} (Si NWs)

Top Down (Wet and dry etching)
**Realizing Si Nanowire: Top down**

### Top down approach: Wet etching

### Bottom Up: CVD process

**Main Advantages** wet chemistry
- No need for special equipment's
- Fabricating Si NWs in a few minutes
- Large areas (4 inch)
- High aspect ratio
- Diameter of sub-micro

Realizing Si Nanowire

Top down approach: Wet etching
(two step process)

Step 1
(5-60)s
Solution 1 (masking)
AgNO₃/HF

Step 2
(0.5-60)min
Solution 2 (etching)
H₂O₂/HF

Main Advantages
- No need for special equipment's
- Fabricating Si NWs in a few minutes
- Large areas (4 inch)
- High aspect ratio

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Top down approach: Wet etching (two step process: step II – Etching time)

5min

30min

70min

Titled image

4 inch Si wafer

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Nano local electrochemical reaction

**Cathode Reaction:**

\[ 4Ag^+ \rightarrow 4Ag_{(s)} + 4h^+ \]

**Anode Reaction:**

\[ Si_{(s)} + 2H_2O + 4h^+ \rightarrow SiO_2 + 4H^+ \]

\[ \text{down arrow} \ 6HF \]

\[ H_2SiF_6 + 2H_2O \]

**Total Reaction**

\[ Si_{(s)} + 4Ag^+ + 6HF \rightarrow 4Ag_{(s)} + H_2SiF_6 + 4H^+ \]
Top down approach: Wet etching
(the mechanism)

Nano local electrochemical reaction

**Cathode Reaction:**

\[ 4\text{Ag}^+ \rightarrow 4\text{Ag}_{(s)} + 4\text{h}^+ \]

**Anode Reaction:**

\[ \text{Si}_{(s)} + 2\text{H}_2\text{O} + 4\text{h}^+ \rightarrow \text{SiO}_2 + 4\text{H}^+ \downarrow 6\text{HF} \]

\[ \text{H}_2\text{SiF}_6 + 2\text{H}_2\text{O} \]

**Total Reaction**

\[ \text{Si}_{(s)} + 4\text{Ag}^+ + 6\text{HF} \rightarrow 4\text{Ag}_{(s)} + \text{H}_2\text{SiF}_6 + 4\text{H}^+ \]
Chapter 2
Surface Treatment & Characterization

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Surface Modification

Molecules on Surfaces (Grignard Reaction, Electrografting)

Phase Transfer (From Cubic to Wurtzite)

Molecules

Direct Laser Writing


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Molecules on Surfaces: Grignard Reaction

- Characterization?
- Replacing oxide shell?
- Si-C bonds?
- Maximum Coverage?
- Stability?
- Oxidation Mechanism

Two Steps Reaction

\[ \text{SiO}_2 \xrightarrow{\text{HF (30 sec)}} \text{Si} \xrightarrow{\text{PCl}_5 (10 \text{ min})} \text{Si} \xrightarrow{\text{RMgCl (2-24 hr)}} \text{Si} \]

Si2p & C1s of Terminated Si NW

Before Alkylation

Si2p

Si2p & C1s of Terminated Si NW

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Impact on Density of State (DOS)  
*In Suite Measurements*

We followed the DOS by using the following:

1. Emission of Si2p
2. Photo-electron Yield (PYS)
3. Work-Function

![Band diagram of CH₃-SiNW, H-SiNW and SiO₂-SiNW surfaces. All the numbers are in eV unit.](image)

\[ \chi_s = \Phi - E_g + (E_F - E_V) \]
\[ \delta = \chi_s - \chi_B \]

<table>
<thead>
<tr>
<th></th>
<th>Si2p</th>
<th>EF-EVBM</th>
<th>( \Phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>99.77</td>
<td>0.83</td>
<td>4.32</td>
</tr>
<tr>
<td>H</td>
<td>99.70</td>
<td>0.98</td>
<td>4.26</td>
</tr>
<tr>
<td>CH₃</td>
<td>99.55</td>
<td>1.05</td>
<td>4.22</td>
</tr>
</tbody>
</table>

Photoemission of Hybrid Si NW

\[ d = 100 \text{ nm} \]

\[ h\lambda = (2-6 \text{eV}) \]

\[ \lambda = 10 \text{nm} \]

\[ \text{Si NW} \]

\[ \text{C} - \text{Si} - \text{H} \]

\[ g_{oc} = \text{occupied density of states} \]

\[ E_{VL} = \text{Vacuum Level} \]

\[ \hbar\omega = \text{optical excitation} \]

\[ g_{oc}(E_{VL} - \hbar\omega) \propto \frac{dY}{d(\hbar\omega)} \]

\[ E_C = \text{Conduction band} \]

\[ E_V = \text{Valence band} \]
Chapter 3: Devices

Solar Cells
Projects: Brief Summary

Surface modifications
Devices: FETs, Solar Cells, Diodes & Transparent electrodes

Publications:

M. Y. Bashouti, BGU, 26.09.2016
Hybrid Solar Cells: PEDOT:PSS/ Si NW


M. Y. Bashouti, BGU, 26.09.2016
Hybrid Solar Cells: PEDOT:PSS/ Si NW


M. Y. Bashouti, BGU, 26.09.2016
Hybrid Solar Cells: PEDOT:PSS/ Si NW

Transparent electrodes

Summary

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Thank you for your attention!