Electronic Transport in Molecular Scale Devices

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I. Electronic Transport of Micro & Nano Via-hole Structures for Molecular Electronic Devices

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Formation of Alkanethiol Self-Assembled Monolayers

Standard alkanethiol molecule

- Octanethiol (C8) $- \text{CH}_3(\text{CH}_2)_7\text{SH} / \text{length} = 13.3\text{Å}$
- Dodecanethiol (C12) $- \text{CH}_3(\text{CH}_2)_{11}\text{SH} / \text{length} = 18.2\text{Å}$
- Hexadecanethiol (C16) $- \text{CH}_3(\text{CH}_2)_{15}\text{SH} / \text{length} = 23.2\text{Å}$

Conjugated molecule: Oligo(phenylene ethynylene) (OPE)

Self-assembled monolayer (SAM)

- A spontaneous chemisorption process
  \[ \text{RS-H} + \text{Au} \rightarrow \text{RS-Au} + 0.5 \text{H}_2 \]
- Chemical bond formation of functional end groups of molecules with the substrate surface
- Intermolecular interactions between the backbones

Reed & Tour, Am. Sci. June 2000
Fabrication of Planar-type Via-Hole Molecular Devices

Design and Fabrication of molecular electronic devices

**Mask pattern**

<table>
<thead>
<tr>
<th>Unit</th>
<th>Die</th>
<th>Devices</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 cm</td>
<td>2.5 mm</td>
<td>190 µm</td>
</tr>
</tbody>
</table>

**Schematic of device**

- One unit contains 16 dies
- Each die contains 20 devices
- Total devices are 320 in a unit

**SEM / AFM / Optical images**

- 4” wafer
  (Collaboration with ETRI, Dr. Hyoyoung Lee)
- 1 cm piece
- Die
- Devices
- AFM image of a device
- After Top electrode

**Fabrication of Planar-type Via-Hole Molecular Devices**

- Optical lithography: ~ 2 µm
- Plan: E-beam lithography: ~ 50 nm

TW Kim, HW Song, GW Wang

Gwangju Institute of Science and Technology

The 3rd Korea-US Nano Forum, Seoul, April 3-4, 2006
1. Yield of molecular devices?
2. How to define working molecular devices?

Device yield (micro-via hole molecular devices)

<table>
<thead>
<tr>
<th># of fabricated device</th>
<th>Fab. failure</th>
<th>short</th>
<th>Open</th>
<th>Working</th>
</tr>
</thead>
<tbody>
<tr>
<td>13440</td>
<td>392</td>
<td>11744</td>
<td>1103</td>
<td>84</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>57</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
</tr>
<tr>
<td>100%</td>
<td>2.9%</td>
<td>87.4%</td>
<td>8.2%</td>
<td>1.5%</td>
</tr>
</tbody>
</table>

Simmons tunneling fitting results for all working devices

<table>
<thead>
<tr>
<th>Alkanethiol</th>
<th>J at 1 V (A/cm²)</th>
<th>( \Phi_B ) (eV)</th>
<th>( \alpha )</th>
<th>( \beta ) (Å⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C8</td>
<td>78000±46000</td>
<td>1.29±0.49</td>
<td>0.76±0.09</td>
<td>0.87±0.16</td>
</tr>
<tr>
<td>C12</td>
<td>2000±400</td>
<td>1.26±0.08</td>
<td>0.72±0.04</td>
<td>0.83±0.04</td>
</tr>
<tr>
<td>C16</td>
<td>5.2±4.7</td>
<td>2.67±0.28</td>
<td>0.52±0.04</td>
<td>0.87±0.05</td>
</tr>
</tbody>
</table>

Representative devices determined by Gaussian fitting of J!
Determination of Working Molecular Devices

Gaussian fitting (3σ: 99.7%)

\[
f(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot e^{-\frac{(x-\langle x \rangle)^2}{2\sigma^2}}
\]

Summary of Log(J)
II. Molecular Electronic Junctions Studied by Conducting Atomic Force Microscopy

Hyunwook Song
Charge Transport Study by CAFM

Au(20nm)/Cr(20nm) coated AFM Probe

HP 4145B

Physical contact area

PSIA, XE-100 model ambient AFM

Chemisorbed Au

C8 OPE
Force-and Length-Dependent Tunneling

I(V) for C12 (1 to 30 nN)

J @ 1 V (1 to 30 nN)

- Larger current with larger loading force
- J: C8 > C12 > C16
- Error bar: sample-to-sample variation

Exponential dependence

\[ R \propto \exp(\beta d) \]
Through-bond vs. Through-space

Tunneling distance in “through space” = \(d - d_{cc}\tan\theta + d_{cc}\)

\[I_t = I_0 \exp(-\beta_{tb} L_M) + \frac{L_M \cos\theta}{I_0} \sum_{N=1}^{d_{ss}} \frac{n_s!}{(n_s - N)!N!} \exp(-\beta_{tb}(L_M - N d_{cc} \tan\theta)) \times \exp(-\beta_{ts} N d_{cc})\]


- The dominant transport mechanism of alkanethiol SAM: “through-bond” tunneling
- When tilted considerably, chain-to-chain coupling: “through-space tunneling” appears
C8: Thru-bond + Thru-space (Single hopping: N = 1)

\[ N \approx 1 \quad (N \leq L_M \cos \theta/d_{cc}) \]
C12: Thru-bond + Thru-space (Double hopping: \( N = 2 \))

\[
\ln \left( \frac{J}{J_0} \right) = -2 \cos \theta \cos \frac{\theta}{2}
\]
C16: Thru-bond + Thru-space (Triple hopping: N = 3)

\[
\ln \left( \frac{J}{J_0} \right) = N \sim 3 \quad (N \leq L M \cos \theta / d_{cc})
\]
Conclusions

- Electronic transport study by CAFM
  - Tip-loading force effects on molecular structural properties
  - Thru-bond vs. thru-space transport

- Fabrication and characterization of micro-via hole molecular devices
  - Detail yield study ~ 1.5 % (out of > 13,000 devices measured)

- Electronic properties of various nanoscale building blocks