Electron Mobility and X-Ray Diffraction of Silicon Phthalocyanine Derivatives in Organic Thin-Film Transistors

Kusuma Virginna Adiningtyas¹,², Owen A. Melville², Benoît H. Lessard²,*

¹Department of Chemistry and Biomolecular Sciences, Faculty of Science, University of Ottawa
²Department of Chemical and Biological Engineering, Faculty of Engineering, University of Ottawa

*corresponding author: benoit.lessard@uottawa.ca

Introduction
Over the years, organic compounds have been incorporated into electronic devices, such as circuitry and computer displays, in the form of organic thin-film transistors (OTFTs). Numerous studies have also been conducted to study the applications of silicon phthalocyanine (SiPc) derivatives. Interest in SiPcs has increased due to their stability, ease of synthesis, and high charge transport. In addition, they can also be chemically modified to be used on flexible surfaces, making them compatible with multiple substrates and used in non-rigid surface (possible applications include printing OTFTs using specific dyes).

An OTFT consists of three electrodes: a source, drain, and gate electrode. The source and drain electrodes are in contact with the organic semiconductive layer, while the dielectric layer insulates the gate electrode.

Figure 1: a) An organic thin-film transistor, viewed from above.
b) Representation of the components in an OTFT. The gold (Au) source/drain electrodes, in contact with the conductive organic layer (in red), sandwich the silicon oxide dielectric layer (in blue) with the silicon gate electrode (in dark grey).

Methodology

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Silicon dibenzoate phthalocyanine</td>
<td>Silicon dichloride phthalocyanine</td>
<td>Silicon dipentafluorophenoxy phthalocyanine</td>
</tr>
</tbody>
</table>

- Three axially disubstituted derivatives were incorporated as active layers into bottom-gate, bottom-contact (BGBC) OTFTs using vapor deposition at various temperatures. Some substrates were treated to increase mobility.
- Electrical testing was conducted to determine the electron mobility (μ), on-to-off current ratio (I_{on}/I_{off}), and threshold voltage (V_t) of the BGBC OTFTs.
- Stacking and alignment of SiPcs crystals were studied using x-ray diffraction.

Results

The results of the electrical testing showed a high electron mobility (μ) amongst SiPc derivatives with the highest diffraction intensity. Increased deposition temperature induces proper stacking and alignment of the SiPcs into a highly ordered crystalline structure. The adopted geometry maximizes electron movement along the film (from source to drain) through shorter π-π stacking distances, and electron mobility is therefore increased. On the other hand, mobility was found to be optimal at a specific temperature, and deposition above the optimal temperature decreased mobility. Reasons for this drop in mobility has not been determined, but could potentially stem from improper stacking of SiPcs (or lack thereof) on the substrate. In BGBC OTFTs made using 1, mobility was optimal with deposition conducted at 200°C.

Figure 2: X-ray diffraction data for BGBC OTFT made using 1. The diffraction peaks above baseline are caused by crystalline structures forming a film on the substrate.

The same electrical and x-ray diffraction tests were conducted on 2 and 3, where correlation between mobility and diffraction is equally observed.

The threshold voltage is a measure of how much voltage needs to be applied before the OTFT goes from an “off” state to an “on” state. A low V_t indicates that the device can operate effectively without applying a high gate voltage (V_g) due to the ease of movement of electrons from source to drain. Therefore, low threshold voltage can be attributed to higher order crystalline structure. Low V_t is ideal in the application of OTFTs in electronic displays. For example, low voltage OTFTs used for LCD screens in cellphones may improve battery life and make devices more efficient.

Another measure of device performance is the on-to-off current ratio. A higher I_{on}/I_{off} ratio shows that the device can conduct more current once V_g exceeds V_t (i.e. the current at its “on” state is higher than at its “off” state). Therefore, with the minimum amount of bias applied to the gate electrode, high-performance devices should conduct significantly more current and possess higher electron mobility, which suggests the film should be highly crystalline in order to allow higher diffraction.

Figure 3: a) Electron field-effect mobility of BGBC OTFTs made using 1 compared with the total observed diffraction above baseline measured using x-ray diffraction.
b) A visual comparison of the effect of substrate temperature during deposition on the field-effect mobility and diffraction above baseline in two areas on OTS treated substrates.

Conclusion

- Positive correlation between mobility and diffraction
- Higher mobility results in better performance of the OTFT
- There is an optimal temperature associated with the maximum mobility

Future research

- Improving mobility using other combinations of SiPc derivatives and materials
- Study of the optimal substrate temperatures and crystalline structure of SiPcs

Acknowledgments

I would like to thank Dr. Benoît Lessard and Owen Melville for their guidance throughout the project, the Lessard Research Group members for their support, and the Office of Undergraduate Research for providing me with the opportunity to conduct this research.

References