Development of Liquid Crystal Thin Films for Application in Photovoltaics

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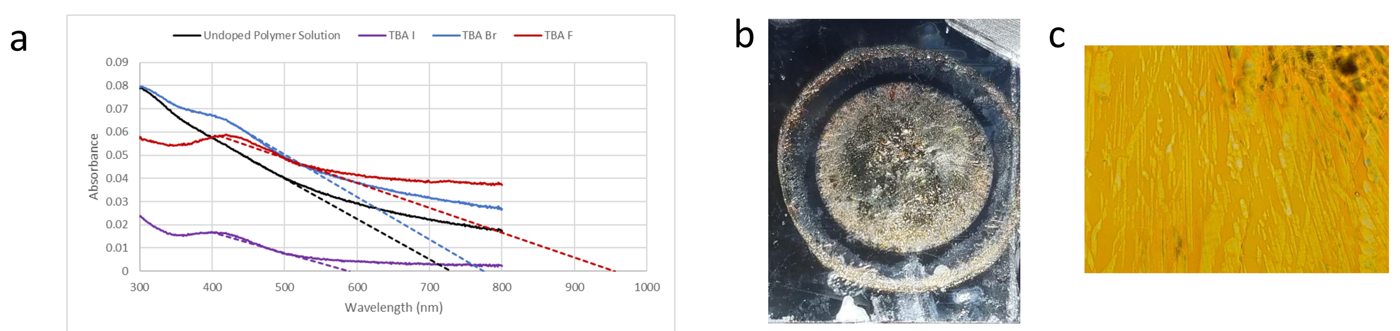
Introduction

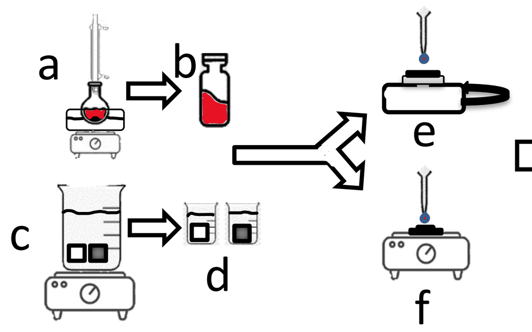
As the world progresses, there is rapid increasing energy demand and urgency to cut down on greenhouse gases; renewable and clean energy technology, such as solar, are in demand for a solution. Silicon derivatives of solar cells are currently the most commercially viable option, but other types, such as organic, perovskite, and multijunction [1], are currently being researched and steadily growing in efficiency. Organic photovoltaics (OPVs) are cost–effective in manufacturing [1 and 2], more durable than other materials [1 and 2], and less difficult to develop films of [2]. One form of organic molecule of particular interest in photovoltaics are organic liquid crystals (OLCs), which present a high amount of order and range of customizability, not only in their macroscopic ordering but also microscopic ordering [2]. Some of the downsides is their current low efficiencies [2] and are sensitivity to impurities in LC phases.

Prior Work



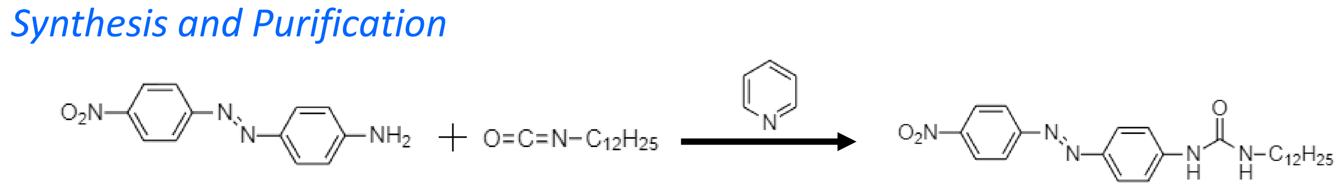
- UV-Vis spectra shows optical band gaps of LC thin films with undoped and doped solutions with tetrabutyl ammonium halides(TBAX, X=F, Br, I), having a tunable range of 1.3-2.1Ev
- Polymer solution doped with TBA Br drop casted on Octadecyl trichlorosilane (OTS) coated substrate (b and c) observe to have best ordering and uniformity

Overall Experimental Design



Characterization: Structural, Optical, Morphological, and Electrical

(a) Synthesis and Purification



- Dr. Cohn laboratory adapted procedure from Ros-Lis et al. [3] in synthesis of polymeric LC product seen in scheme 1. Several purification techniques used.

Thin Film Development

- (b) Solution Development
  - High Boiling Point Co-Solvent (0.4:0:6 molar Diphenyl Ether:THF)
  - Tuning with different equivalents of TBA Br
- (c) Cleaning Substrates
  - Alconox, Acids and Bases [4], Organic Solvents [5]
- (d) Increasing surface attraction with surfactant coating
  - Dip-coating OTS adapted from XU and Ko [3] and Banga et al. [4]
- (e & f) Thin film Fabrication
  - Drop casting or Spin Coating
- Characterization
  - UV/Vis Spec, AFM, Conductivity, XRD, Optical Microscope

Results

Synthesis and Purification of LC Polymer

- Synthesis did not scale up to produce a significant product yield
- 1-dodecylisocyante was impure
- Several impurities in the crude reaction mixture
- Pyridine/Pyridinium salts, DO3, and carbamic acid byproduct
- Several purification techniques with differing purity obtained, never 100% purity
- Flash column and heating gently to evaporate solvents had the best purity

LC Thin Film Development

- All OTS dip coated films produced from all methods of cleaning were clear visually, but only substrates cleaned with boiling isopropanol were able to be become wet by THF or the polymer solution

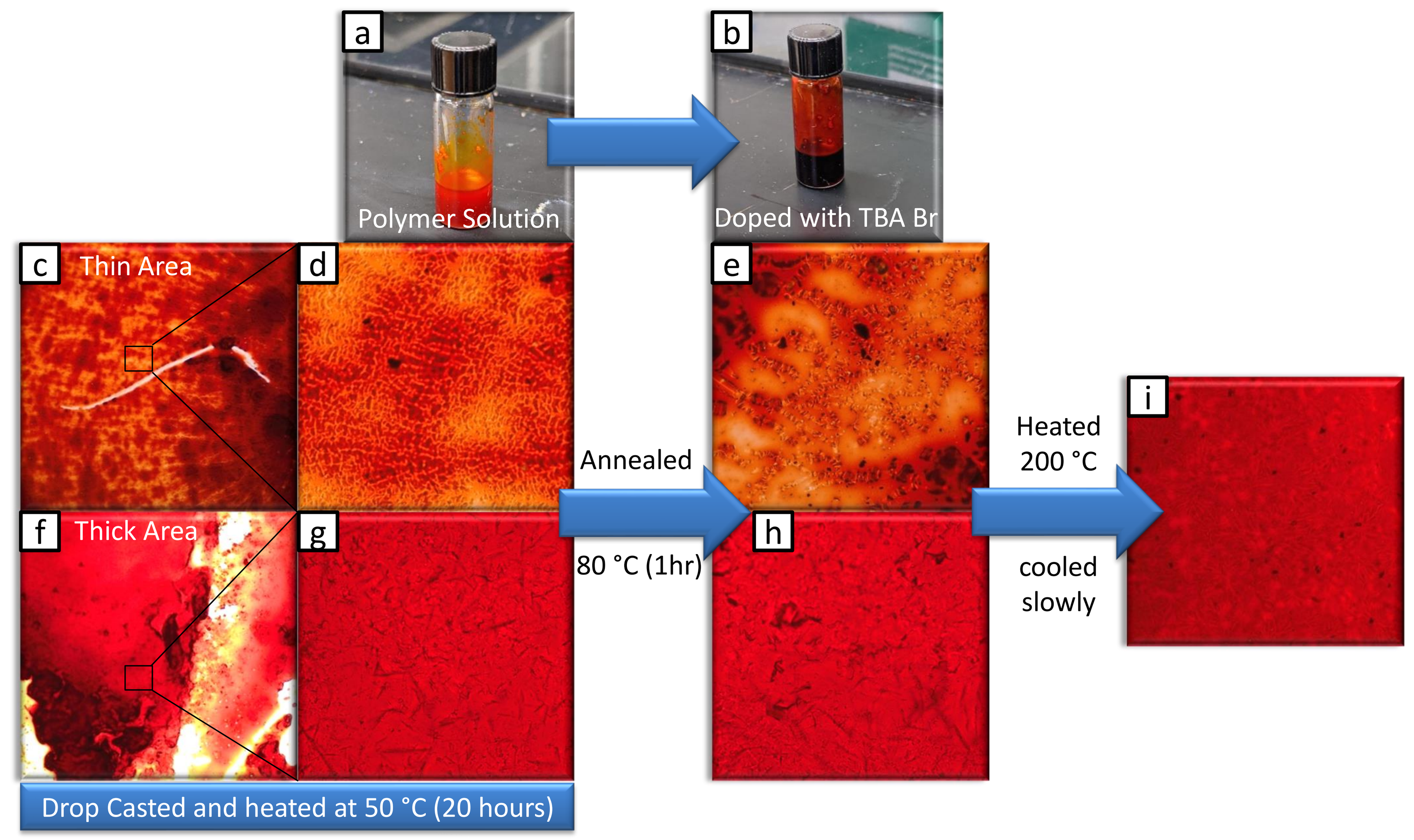


Image Series 1

- A crude polymer solution used for drop casting (b) this specific film is shown before (a) and after (b) adding TBA Br, going from orange to deep red
- Thin spots had a random cracked crystalline pattern, being both red and orange/yellow and thick spots have a random but uniform red crystalline pattern
- Heating/Annealing the film at differing temperatures changes the order of the film since the LC phases of the polymer at observed at 80 °C and 120 °C, and at the liquid phase (200 °C) the film became homogenous and organized

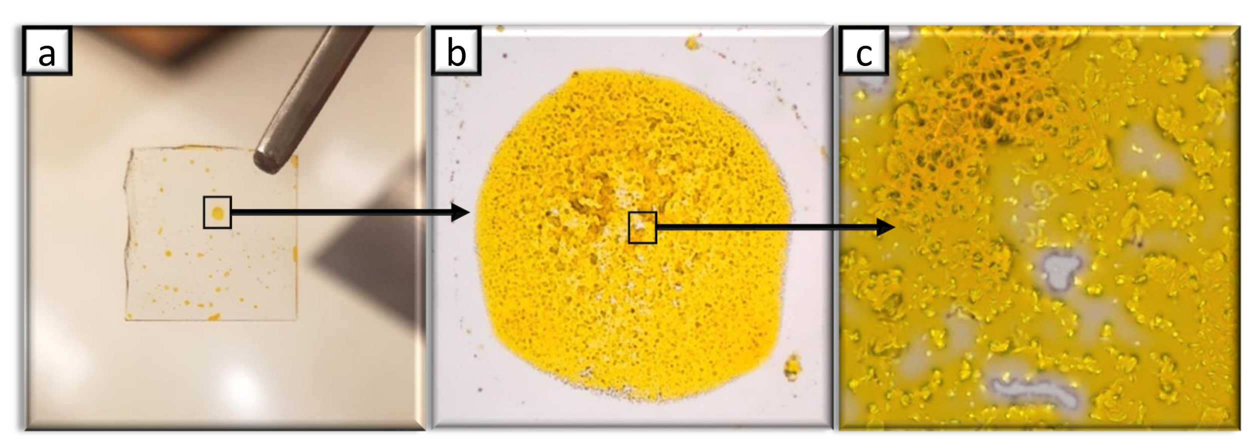
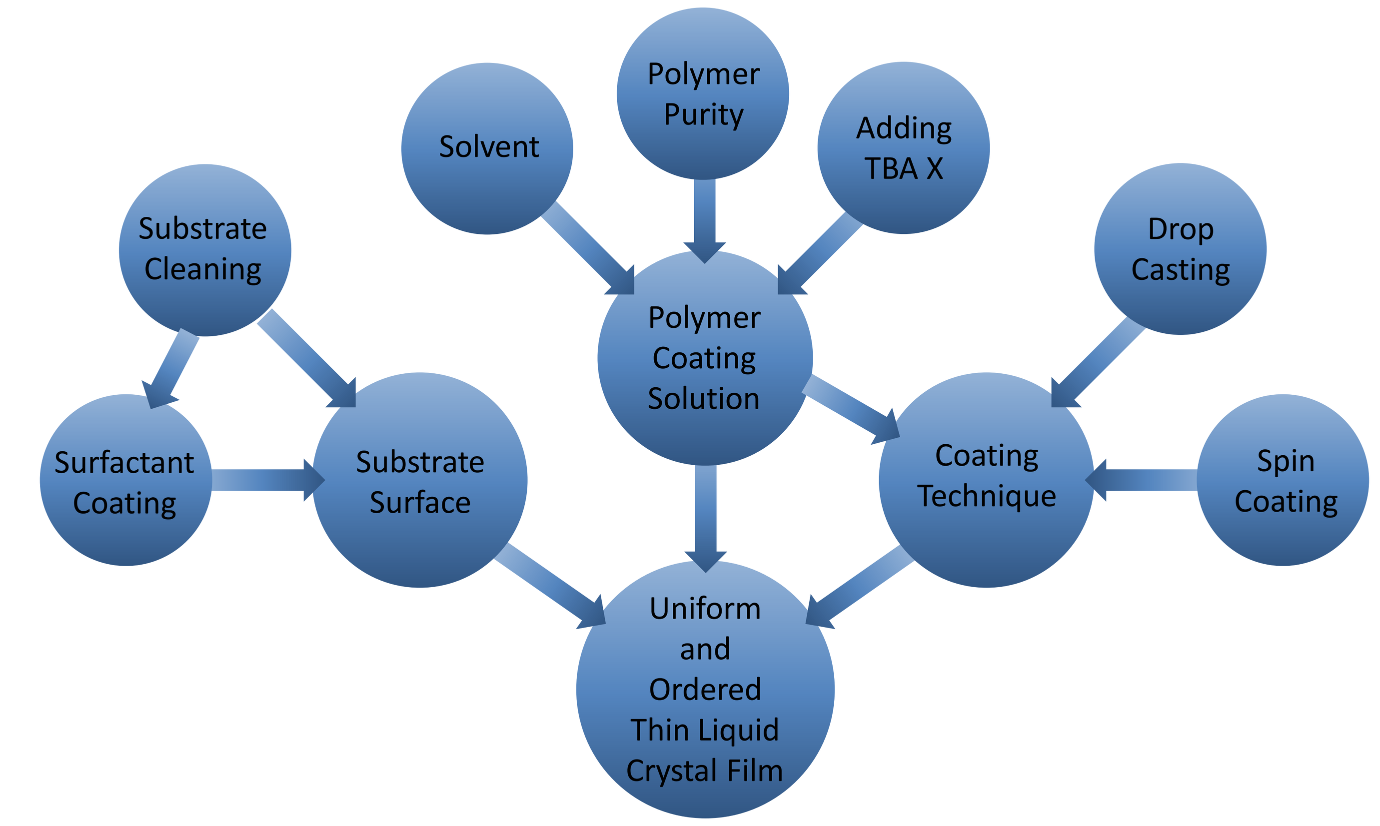


Image Series 2

- Image Series 2 shows a "film" that was spin coated with a solution of majority pure polymer with TBA Br
  - Substrate cleaned using water, other organic solvents and then dip coated in OTS
- The solution did not wet sufficiently on the substrate, having a "hydrophobic affect."
- The porous spot observed focused on image series 2 may be caused by rapid solvent evaporation when drying, further proving the wide range a variability in LC polymer film

Conclusions



Synthesis and Purification of LC Polymer

- Due to 1-dodecylisocyante stock impurities all products contained a carbamic acid byproduct
- Difficulty of scaling up the synthesis reaction and purification

LC Thin Film Development

- Polymer solution color is sensitive adding TBA Xs
- Ideal technique for cleaning substrates was with boiling isopropanol, while other techniques didn't allow sufficient OTS coatings
- Thin films sensitive to initial substrate surface, coating solution, coating technique, and temperature.
  - Difficulty in fabricating a continuous film

Future Plans

- Optimize thin film fabrication methods (explore dip coating)
- Characterize uniform and ordered films with AFM, UV/Vis Spectroscopy, XRD, and Conductivity

References

[1] Solar Energy Technologies Office. Solar Photovoltaic Cell Basics. (https://www.energy.gov/)

[2] Kumar, M.; Kumar, S. Liquid Crystals in Photovoltaics: A New Generation of Organic Photovoltaics. *Polymer Journal* **2017**, *49* (1), 85–111.

[3] Ros-Lis, J. V.; Martínez-Máñez, R.; Sancenón, F.; Soto, J.; Rurack, K.; Weißhoff, H. Signalling Mechanisms in Anion-Responsive Push-Pull Chromophores: The Hydrogen-Bonding, Deprotonation and Anion-Exchange Chemistry of Functionalized Azo Dyes. *Eur. J. Org. Chem.* **2007**, *2007* (15), 2449–2458.

[4] XU, G.-hua; Ko, H. Formation of OTS Self-Assembled Monolayer on Glass Surface Investigated by AFM. *Journal of Zhejiang University Science* **2000**, 1 (2), 162.

[5] Banga, R.; Yarwood, J.; Morgan, A. M.; Evans, B.; Kells, J. FTIR and Afm Studies of the Kinetics AND Self-Assembly of Alkyltrichlorosilanes And (Perfluoroalkyl)Trichlorosilanes Onto Glass and Silicon. *Langmuir* **1995**, 11 (11), 4393–4399.

Acknowledgments

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