Modeling Substrate Patterning for Organic Photovoltaics Using Computational Systems

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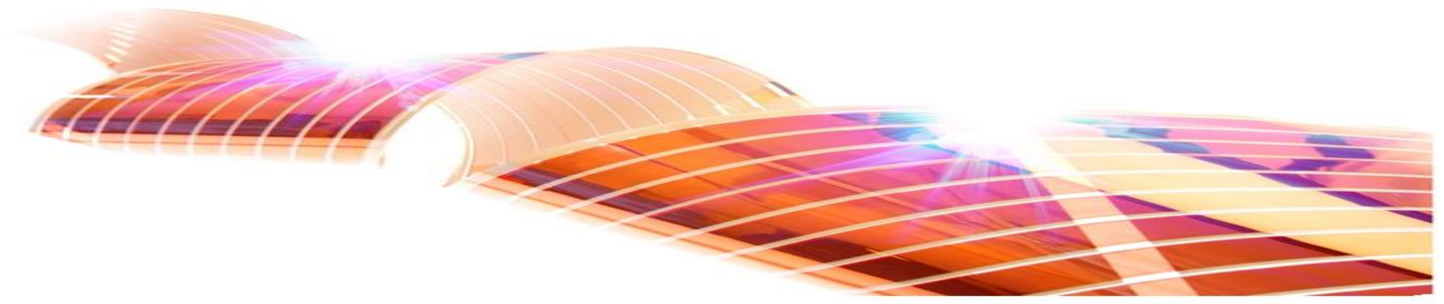
Introduction

- More sustainable and readily available sources of energy are necessary to meet increasing demands
- Organic photovoltaics (OPVs) – thin film (~100 nm) polymer-fullerene blended cells that utilize sunlight to generate electricity
- Advantages of OPVs over inorganic solar cells
  - Flexible
  - Easy to mass-produce through roll-to-roll printing
  - Inexpensively manufactured
- Challenges that need to be addressed
  - 4.2% to 10% efficiencies (low) [1]
  - Expensive - estimated costs around \$7.85/m² [2]
    - *Payback period of approximately 20 years* [2]
  - Limited lifespans

Figure 1: Car coated with spray-on OPV cells



Project Motivation and Objectives

- Improving microstructure can enhance free charge separation
  - Increases structural order
  - Creates predictable pathways for separation
- Objectives:
  - Understand how different microstructures form during solvent evaporation in 2D
  - Identify different modes and understand differences between non-substrate patterned systems vs. those with substrate patterning
  - Identify ideal substrate patterning to optimize organic photovoltaic efficiency in a PS/PMMA system

Figure 2: System without substrate patterning

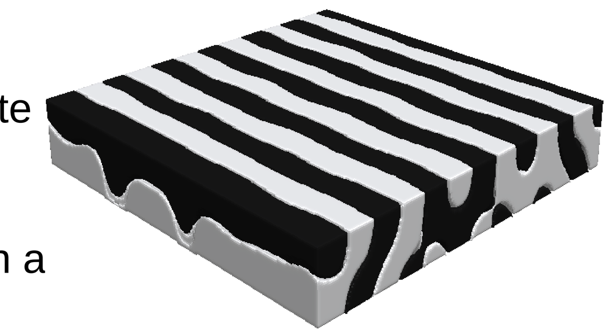
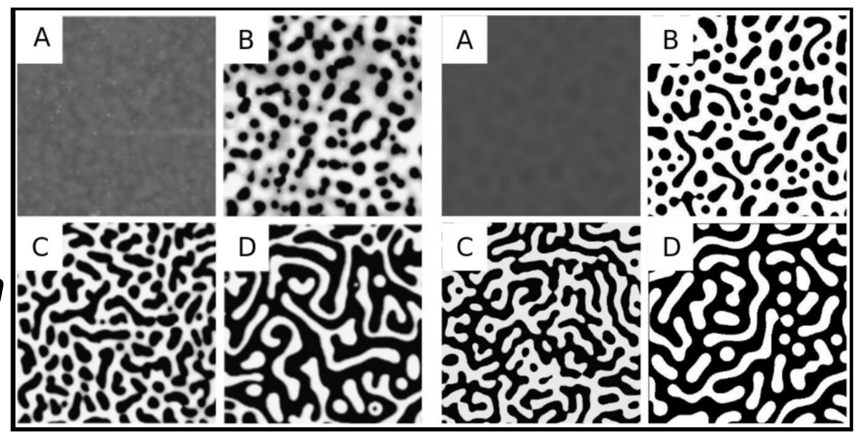


Figure 3: System with substrate patterning

Methodology and Framework

- MESC (Morphology Evolution during Solvent-based Coating): experimentally validated three-dimensional element-based framework [3]
  - Models microstructure evolution due to:
    - *Solvent choice and evaporation*
    - *Blend ratio*
    - *Degree of polymerization*



Experimental Computational

Results and Discussion

- Biot number:
  - Ratio between solvent evaporation from surface to internal diffusion of solvent within the bulk material
  - Equation: $Bi = \frac{k_e}{D_s/L}$
- Blend ratio
  - Ratio of polymer to fullerene (PS to PMMA)

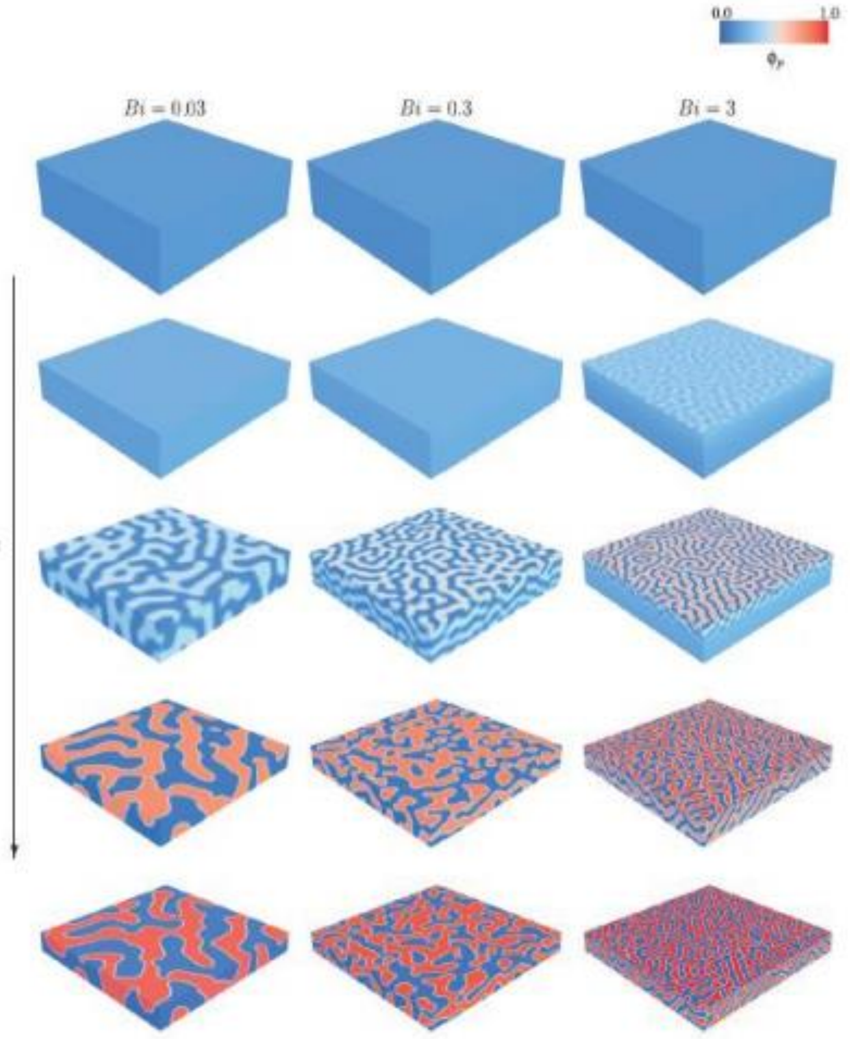
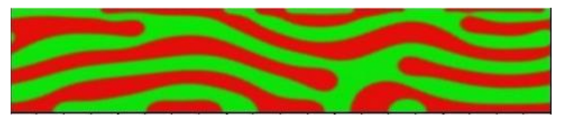


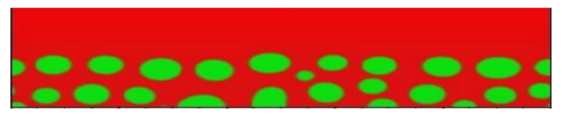
Figure 4: Effect of Biot number on a polymer system. A lower Biot number (left) represents a system dominated by diffusion and results in more coarsened regions and slower evaporation. A higher Biot number (right) represents a system dominated by evaporation and results in smaller domain sizes and faster evaporation.

- Four established modes

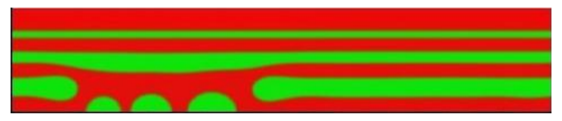


- ***M1*** – Phase separation beginning from top surface (thin, interconnected pathways)

- ***M2*** – Spontaneous phase separation throughout system (medium thickness, interconnected pathways)



- ***M3*** – Phase separation below top layer (islands)



- ***M4*** – Phase separation initiated from the bottom surface (layers)

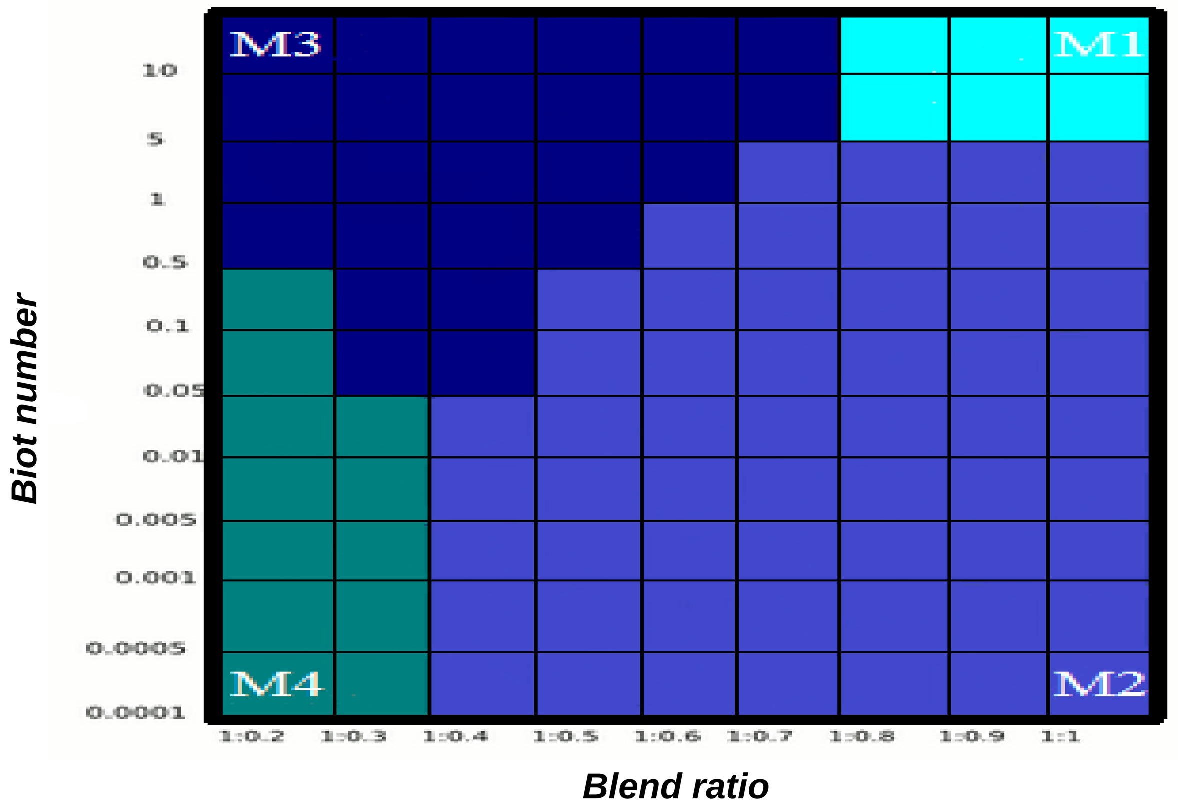


Figure 5: Morphology map of the different modes without substrate patterning. M1 typically occurs with similar or equal amounts of both polymer and fullerene and at higher Biot numbers. M2 occurs in a wide range of blend ratios but at lower Biot numbers than M1. M3 occurs when blend ratio is unbalanced and when the Biot number is large. M4 occurs when blend ratios are unbalanced and with lower Biot numbers.

Results and Discussion

- Substrate patterning leads to changes in microstructure
  - Substrate can be patterned alternately with one material that is attractive to polymer and another that is attractive to fullerene
    - *Note checkered microstructure and orientation of polymer to substrate patterning*
    - *Tendency to layer when bulk domain size does not match substrate patterning domain size*
    - *Coarsening leads to thicker domain sizes that are not influenced as strongly by substrate patterning*

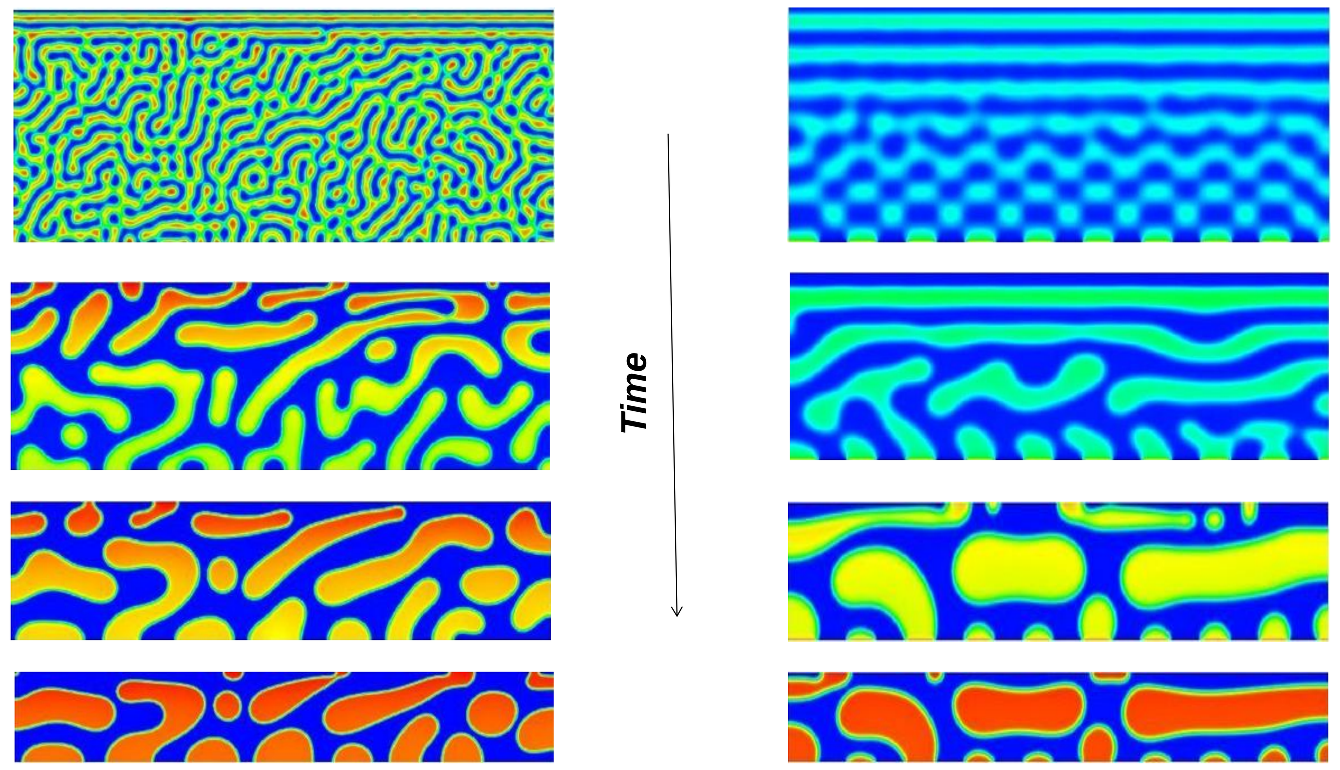


Figure 6: Systems with identical parameters (Blend ratio – 1:1, Biot number – 1). No substrate patterning (left) and substrate patterning (right).

Conclusions

- **Benefits of computational frameworks:**
  - High thorough-put analysis
  - Isolate material specific parameters and assess the relative sensitivity upon the resultant OPV microstructure
- **Substrate patterning can be included in computational models to simulate real laboratory practices such as nanoimprint lithography, microcontact printing, and dip-pen nanolithography**
  - Identify advantages and disadvantages of substrate patterning
  - More accurately model OPV creation process

Future Work

- **Understand how modes change when substrate patterning is added to a system and generate an altered morphology map**
- **Design optimal substrate patterning scheme that may be used to produce highly ordered microstructures for a wide variety of materials**

References

1. Green et al. (2012). Solar cell efficiency tables (version 39), 12–20.
2. Mulligan et al. (2014). A projection of commercial scale organic photovoltaic module costs. *Solar Energy Materials and Solar Cells*, *120*, 9–17.
3. Wodo et al. (2012). Modeling morphology evolution during solvent-based fabrication of organic solar cells. *Computational Materials Science*, *55*, 113–126.

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