A computational model for growth of thin organic semiconductor films

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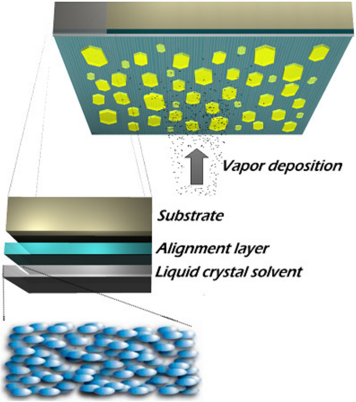
Outline

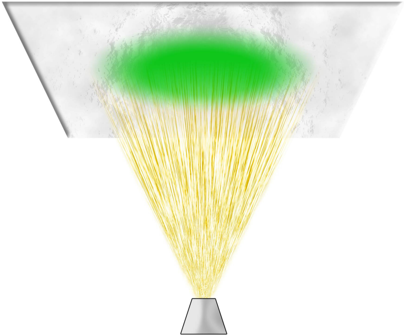
- the experiment
- the model
- scaling theory
- results from simulation
- future work

The Experiment

- organic semiconductor heated and evaporated
- vapor deposited onto substrate
- particles diffuse and form islands



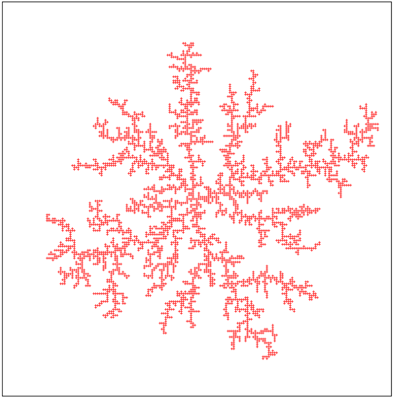
Forced Deposition



- vapor propelled out of a nozzle
- large velocity gradient near substrate
  - boundary layer though which particles must diffuse
- possible aggregation of particles in vapor as they diffuse through boundary layer as well as on substrate
- some sort of cluster growth model is needed...

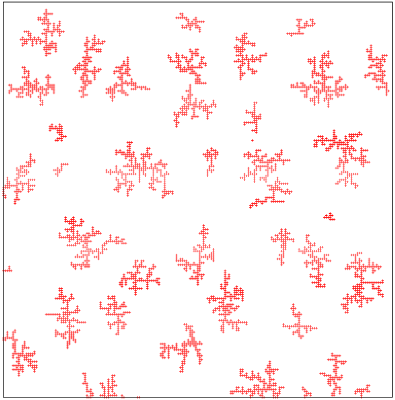
Diffusion Limited Aggregation Model

- start with seed particle
- drop one particle at a time
- let particle walk until it runs into the seed or wanders away
- continue process to grow cluster



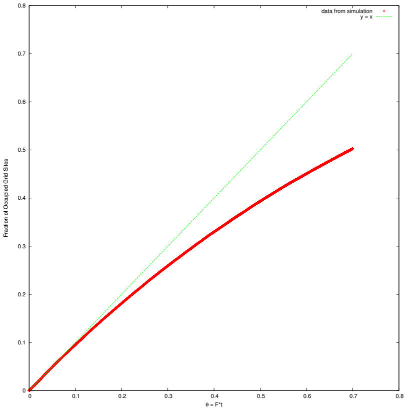
Deposition, Diffusion, Aggregation Model

- deposition: monomers deposited at rate F monomers per unit time per unit area
- diffusion: monomers diffuse with mean time between hops $\tau \sim 1/D$
- aggregation: monomers stick to other monomers
  - form islands
  - islands grow by capture of monomers



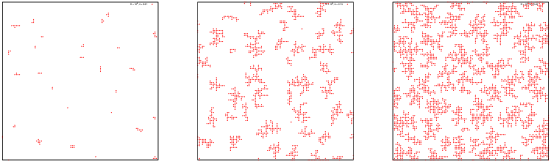
Defining The Coverage

- what do we do when monomers land atop islands or other monomers?
    - let them walk around until they “fall down”?
    - ignore them?
- how do we define coverage?
    - total number of monomers deposited divided by total area?
    - total number of occupied grid sites divided by total number of grid sites?

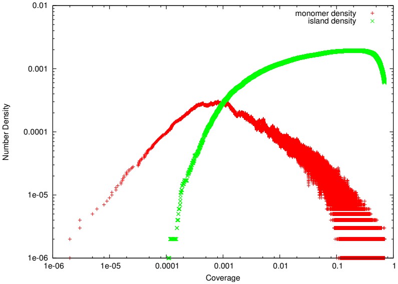


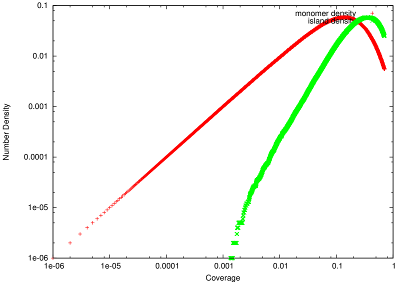
Growth Regimes

- initial deposition
  - monomers few and far between
  - linear increase in monomer density
- aggregation
  - island formation by aggregation of monomers becomes important
  - island density increases and monomer density levels off
- coalescence
  - merging of islands becomes important
  - island density quickly drops

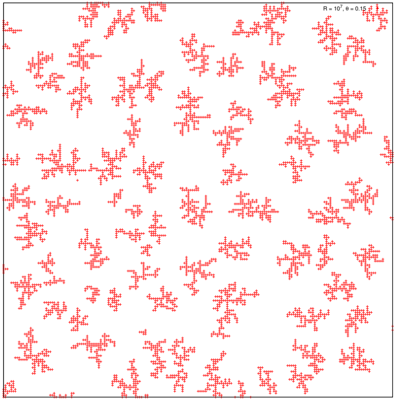


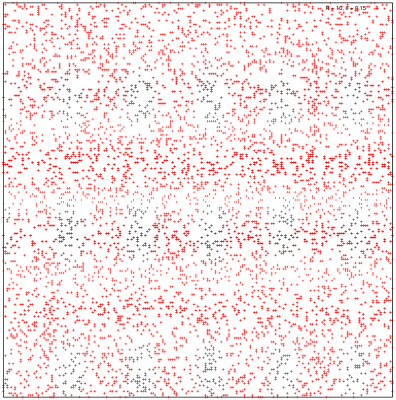
Growth Regimes





Island Morphology





Scaling Theory

- island size distribution can be written in the form:

$$N_s(\theta) = \frac{\theta}{\langle s \rangle^2} f_i \left(\frac{s}{\langle s \rangle} \right)$$

- f_i is a universal scaling function
  - does not depend on coverage
  - does not depend on R, so long as R is large
  - dependent only on critital island size i

In Search Of A Functional Form for f_i...

- assumptions proposed by Amar and Family [?]
  - the island size distribution behaves as u^i for small u
  - the distribution has an exponential cuttoff for large u
  - the distribution peaks at the average island size $(u = 1)$
- leads to the functional form

$$f_i(u) = C_i u^i e^{-ia_i u^{1/a_i}}$$

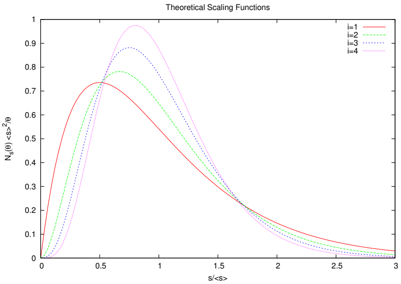
- The constants C_i and a_i are determined by applying the sum rules $\int f_i(u)\ du = \int u f_i(u)\ du = 1$,

$$\frac{\Gamma[(i+2)a_i]}{\Gamma[(i+1)a_i]} = (ia_i)^{a_i}, \quad C_i = \frac{(ia_i)^{(i+1)a_i}}{a_i \Gamma[(i+1)a_i]}.$$

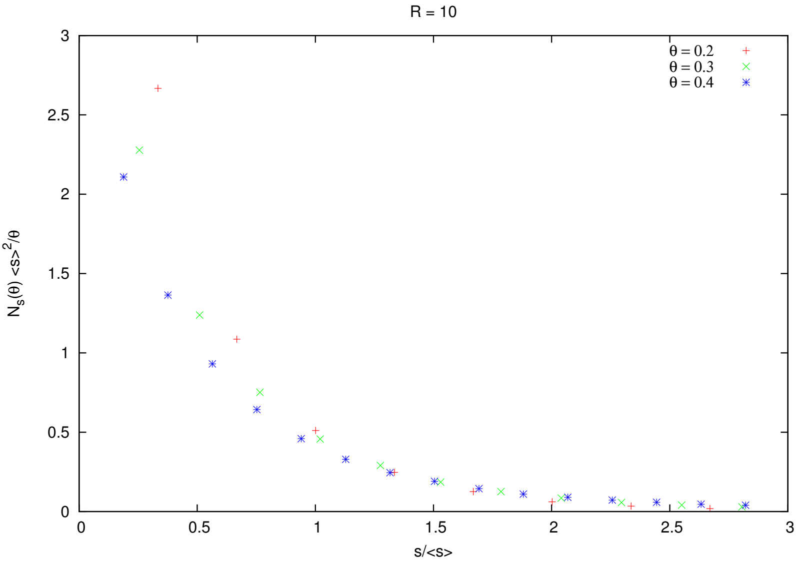
...but is there a better way?

- why assume distribution peaks at $u = 1$?
- lets relax the constraint $u = 1$ and see what we get...
- more simple scaling function $f_i(u) = Au^i e^{-iub}$
- sum rules again fix constants and *BLAM!*

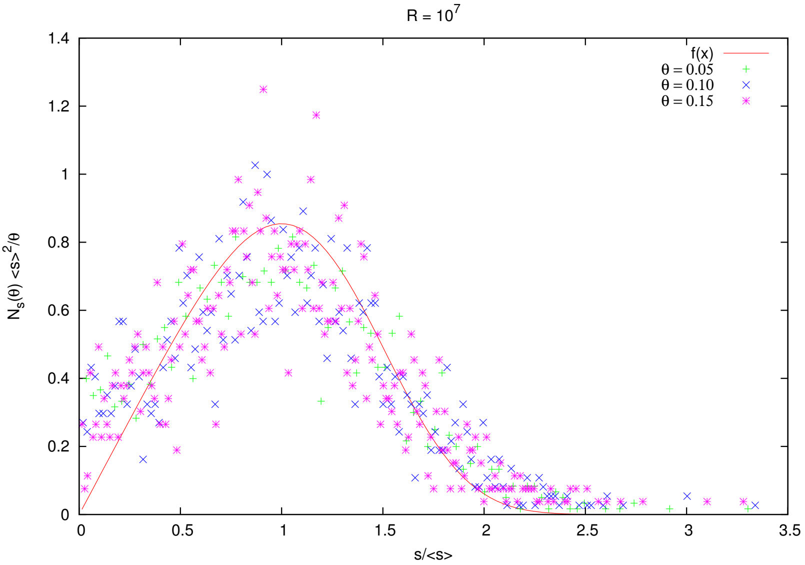
$$f_i(u) = \frac{(i+1)^{i+1} u^i e^{-(i+1)u}}{\Gamma(i+1)}$$



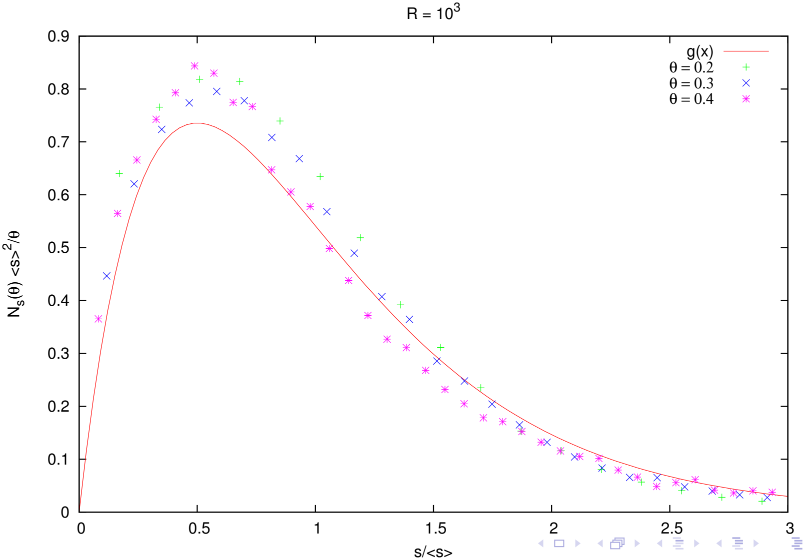
The Small R Regime...



...The Asymptotic Large R Regime...



...The Not So Small, Not So Asymptotic Large R Regime



Future Work

- get to the bottom of two dimensional scaling theory for $i = 1$
- investigate scaling theory for $i > 1$
- deposition of clusters
- extend model to three dimensions
  - diffusion through boundary layer
  - diffusion through liquid crystal layer

References

- Jacques G. Amar and Fereydoon Family, Phys. Rev. Lett. **74**, 2066 (1995)
- J.A. Blackman and P.A. Mulheran, Phys. Rev. B. **54**, 11 681 (1996)
- Pablo Jensen, Rev. Mod. Phys. **71**, 1695 (1999)