A Computational Model For Growth Of Thin Organic Semiconductor Films

Benjamin R. Hillman, Brad L. Johnson

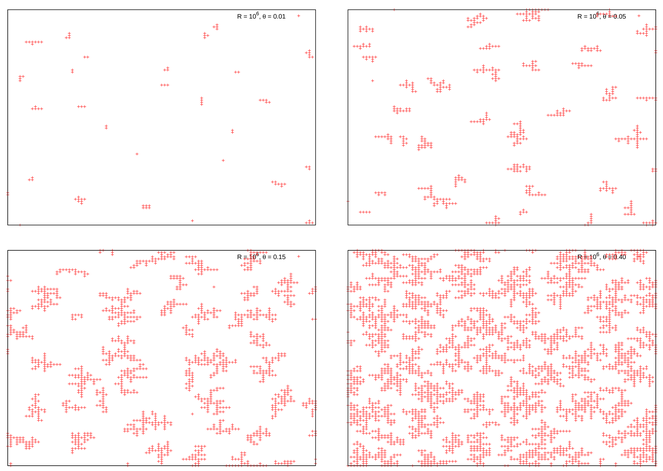
Department of Physics and Astronomy, Western Washington University

Introduction

We are investigating a new method of growing thin organic semiconductor films which incorporates a forced deposition of organic vapor onto a substrate. Particles in the vapor can diffuse and aggregate both while in the vapor and after they have contacted the substrate. We present here our preliminary work on a computational model to simulate the growth process on the substrate and investigate the scaling behavior of island size distribution in deposition diffusion aggregation models.

The Model

- monomers are deposited onto a grid at a rate of F monomers per unit time per unit area
- monomers diffuse with mean time between hops proportional to $1/D$
- islands form when monomers stick to other monomers and grow as islands capture more and more monomers
- critical island size i corresponds to one less than smallest stable island size
- irreversible sticking corresponds to critical island size $i = 1$ and leads to fractal islands



Scaling Theory

It has been shown that the island distribution function can be written in the form[1]

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

where $N_s(\theta)$ is the number of islands of size s per unit area for a given coverage θ, $\theta = Ft$ is the coverage, s is island size, $\langle s \rangle$ is the average size and f_i is a universal scaling function for a given critical island size i. By universal, we mean that the function is independent of the coverage and of the growth parameters F and D. The scaling function should, however, be different for different critical island sizes i. A functional form of the scaling funciton can be obtained from the following assumptions[1]:

- 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 ($u = 1$)

These assumptions lead to the functional form

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

The constants C_i and a_i are determined by applying the sum rules $\int f_i(u)\, du = \int u f_i(u)\, du = 1$, which arise because the scaling function is really just a probability function [2]. The result of applying the sum rules to the above scaling functional form is

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

We propose a slightly different approach to the scaling function by *not* requiring the distribution to peak at the average island size, as we see no constraint on this peak *a priori*. Keeping the rest of the assumptions leads to the much simpler scaling function $f_i(u) = Au^i e^{-iub}$. Again, the sum rules fix the values of A and b, and the result is the function

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

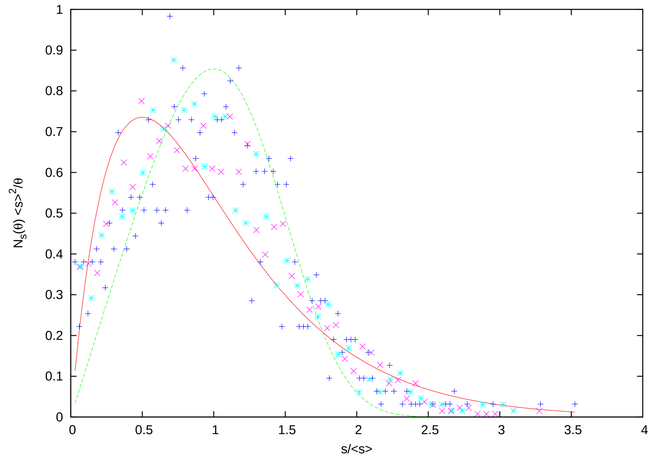
References

[1] Jacques G. Amar and Fereydoon Family, Phys. Rev. Lett. **74**, 2066 (1995)

[2] J.A. Blackman and P.A. Mulheran, Phys. Rev. B. **54**, 11 681 (1996)

[3] Pablo Jensen, Rev. Mod. Phys. **71**, 1695 (1999)

Results from Simulation



The above is a plot of the simulation data along with the two distribution functions described previously. The simulation is a Monte Carlo technique based on an algorithm proposed by Pablo Jensen [3]. The plot contains simulation data for values of $R = D/F$ ranging from 10^3 to 10^6 and for coverages ranging from 0.05 to 0.15.

We see that the large s (large island size) regime is fit well by the newly proposed distribution function; the small s regime is less clear, and more simulation data based on larger grid models is underway. Experimental results will be used to charactize the distribution function as well.

Future Work

More simulation data is needed to resolve the uncertainies seen above in the small s regime. Additionally, work needs to be done to verify the distributions for higher values of the critical island size i.

After verifying the scaling results in two dimensions, we would like to look at the effects of deposition of not just monomers but of clusters as well (dimers, trimers, etc.), corresponding to aggregation occuring in the vapor. Additionally, diffusion through the liquid may become important as well.

Contact information: Benjamin R. Hillman – Phone: 425–218–8086 – Email: benjaminr.hillman@gmail.com