Mean Field Theory of Polynuclear Surface Growth

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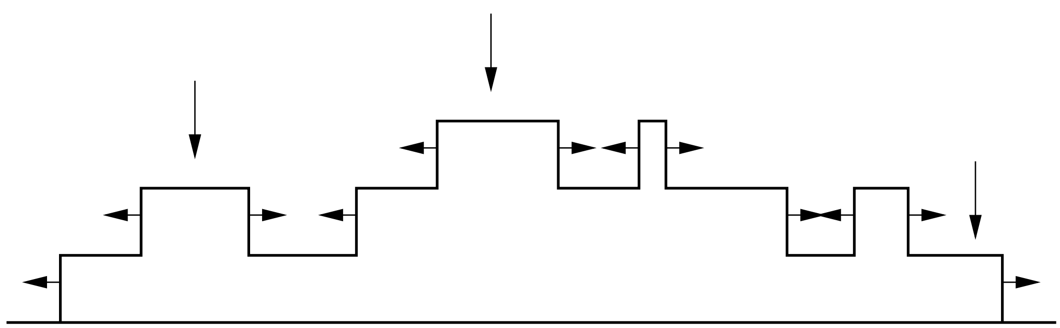

Fig.1 Illustration of the PNG process

I. Polynuclear Growth (PNG)

The Model: Sizeless islands **nucleate** uniformly in space and time with rate γ. Islands **grow** laterally in the radial direction with constant velocity v. Coalescence of islands results in a larger island. The joint perimeter keeps growing in the original radial direction. Set $\gamma = v = 1$, without loss of generality.

Applications (2D): Polymer lammellar crystallization

Equivalent to (1D): Kink-Antikink gas in overdamped sine-gordon equation. Kinks (Antikinks) correspond to up (down) step edges, i.e., $h(x,t) \to dh(x,t)/dx$. Island growth equivalent to ballistic kink motion. Island coalescence corresponds to Kink-Antikink **annihilation**.

Equilibrium properties are known (1D):

— Fluctuations in surface hight scale with system size as $\sim L^{1/2}$

— Surface growth velocity: $v_{\rm eq} = \sqrt{2}$

nonequilibrium (infinite system) properties unknown

The uncovered fraction

$S_j(t)$ = the exposed fraction of the jth layer at time t. Many properties follow directly:

The surface hight, $h(t) \sim vt$

$$h(t) = \langle j \rangle = \sum_{j=1}^{\infty} j \left[S_{j+1}(t) - S_j(t) \right].$$

The surface width, $w(t) \sim t^{\beta}$

$$w^2(t) = \langle j^2 \rangle - \langle j \rangle^2 = \sum_{j=1}^{\infty} j^2 \left[S_{j+1}(t) - S_j(t) \right] - h^2(t)$$

Wave-like asymptotic form

$$S_j(t) = F\left(\frac{j - vt}{t^{\beta}} \right)$$

Extremal properties

$$F(z) \sim \begin{cases} 1 - \exp(-z^{\sigma_+}) & z \to \infty; \\ \exp(-|z|^{\sigma_-}) & z \to -\infty. \end{cases}$$

Large coverage follows a Fisher tail, $\sigma_+ = \frac{1}{1-\beta}$

The gap density

$f_j(x,t)$ = the density of inter-island gaps (voids) of length x on the jth layer. Gives

The uncovered fraction

$$S_j(t) = \int_0^\infty dx\, x\, f_j(x,t)$$

The island density

$$N_j(t) = \int_0^\infty dx\, f_j(x,t)$$

Master equation

$$\frac{\partial f_j(x,t)}{\partial t} = 2\frac{\partial f_j(x,t)}{\partial x} + \gamma_j(t)[-x f_j(x,t) + 2\int_x^\infty dy f_j(y,t)]$$

first term - gap shrinkage due to surface growth

next two terms - changes due to nucleation.

$\gamma_j(t)$ = nucleation rate at the jth layer

implies correct rate equation, $\dot{S}_j(t) = -2N_j(t)$

Island density rate equation

$$\dot{N}_j(t) = -2f_j(0,t) + \gamma_j(t)S_j(t)$$

II. Mean-Field Theory (MFT)

Compare with exact island density rate equation

$$\dot{N}_j(t) = -2f_j(0,t) + S_j(t) - S_{j-1}(t)$$

To comply with this equation, the nucleation rate must be

$$\gamma_j(t) = 1 - \frac{S_{j-1}}{S_j}$$

Formal solution for gap density, $g_j(t) = \int_0^t d\tau\, \gamma_j(\tau)$

$$f_j(x,t) = g_j^2(t)\, \exp\left[-g_j(t)x - 2\int_0^t d\tau g_j(\tau)\right]$$

Uncovered fraction obeys second order nonlinear ODE

$$\frac{d^2}{dt^2}\ln S_j = -2\left(1 - \frac{S_{j-1}}{S_j}\right) = -2\gamma_j$$

$\boxed{\textbf{self consistent nucleation rate}}$

Traveling wave solution

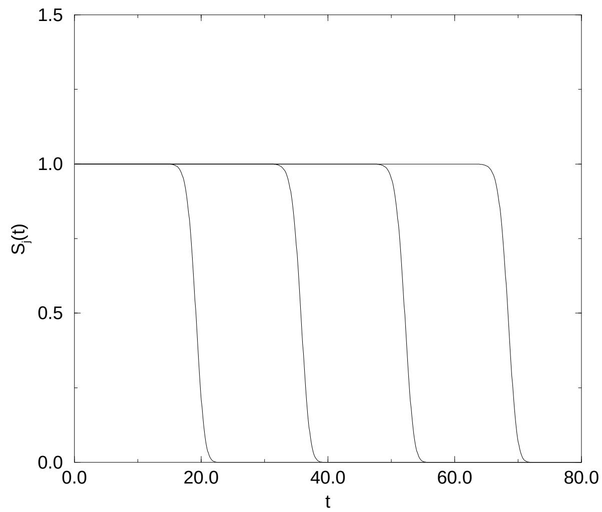

Fig.2 The uncovered fraction $S_j(t)$ vs. time for layers $j = 20$, 40, 60, and 80.

The coverage follows a traveling wave solution, $S_j(t) = F(j - vt)$. For $j \gg vt$, $1 - F(x) \sim \exp(-\alpha x)$ with

$$v^2 = 2\frac{e^\alpha - 1}{\alpha^2}$$

As $\alpha > 0$ all velocities in the range $[v_{\rm min}, \infty)$ are possible. However, the minimal possible velocity is selected and $v = v_{\rm min} = 1.75735$. This agrees to 0.1% with the numerics!

$\boxed{\textbf{minimal stable velocity is selected}}$

Extremal Properties of Coverage

$$F(z) \sim \begin{cases} 1 - \exp(-\alpha z) & z \to \infty; \\ \exp(-z^2) & z \to -\infty. \end{cases}$$

Generalization to higher dimensions

Higher order rate equation

$$\frac{d^{d+1}}{dt^{d+1}} \ln S_j = -d!\Omega_d \left(1 - \frac{S_{j-1}}{S_j}\right) \qquad \Omega_d = \pi^{d/2}/\Gamma(1+d/2)$$

Again, a traveling wave form for $S_j(t)$. All qualitative properties are similar to 1D including asymptotically flat surface, $\beta = 0$

Minimal velocity selected

$$v^{d+1} = d!\Omega_d \, \frac{e^{\alpha} - 1}{\alpha^{d+1}}$$

$$\boxed{\textbf{asymptotically smooth surface predicted}}$$

III. Linear Recursion Relation (LRR) approach

Uses known Kolmogorov coverage in first layer, $S_1(t)$ [2]

$$S_{j+1}(t) = S_j(t) - \int_0^t d\tau \, S_1(t-\tau) \, \frac{dS_j(\tau)}{d\tau}$$

Reduces to diffusion equation

$$\frac{\partial S}{\partial t} = D \frac{\partial^2 S}{\partial z^2} \qquad z = j - vt$$

Growth velocity

$$v_d = \left(\frac{\Omega_d}{d+1} \right)^{\frac{1}{d+1}} / \Gamma \left(\frac{d+2}{d+1} \right).$$

Symmetric wave form, $\mathrm{Erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty du \, e^{-u^2}$

$$S_j(t) = \frac{1}{2} \mathrm{Erfc}(-x) \qquad x = \frac{j - v_d t}{\sqrt{4Dt}}$$

$$\boxed{\textbf{diffusive growth of width } \beta = 1/2}$$

IV. Monte Carlo simulations

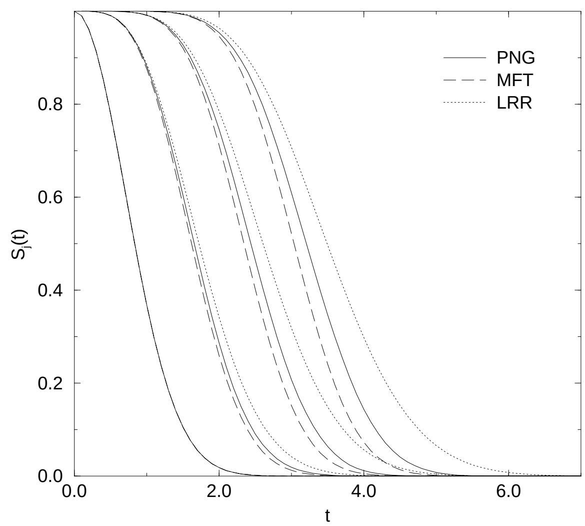

Fig.3 Uncovered fraction $S_j(t)$ versus t for $j = 1, 2, 3, 4$

MFT gives an improved approximation

MFT and LRR provide lower and upper bounds

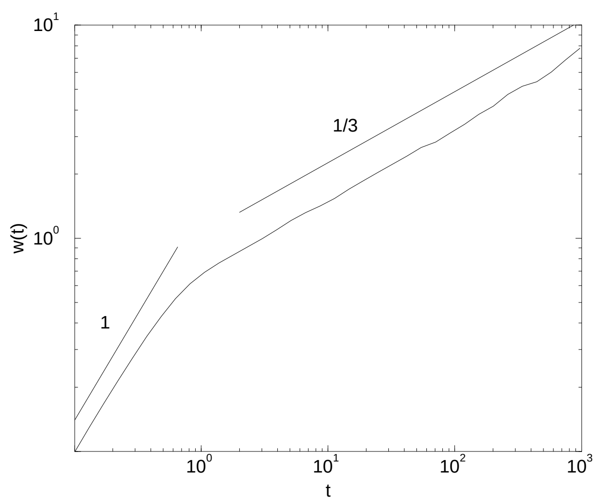

Fig.4 Long time behavior of the width. Early behavior is linear and late behavior is $t^{1/3}$.

1D PNG is in KPZ universality class [5]

Summary

	MFT	PNG	LRR
v_1	1.75735	1.41 ± 0.01	1.12838
β	0	1/3	1/2
σ_+	1	3/2	2
σ_-	2	≥ 2	2

Table 1: Characteristics of the three approaches for the one-dimensional PNG model.

Conclusions

- **MFT provides better approximation for coverage**
- **MFT improves for higher dimensions**
- **MFT and LRR provide upper and lower bounds**

References

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