Geometric Motion in Epitaxial Phenomena

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Outline

Introduction

Epitaxy techniques growth modes

Submonolayer Growth

Island morphologies

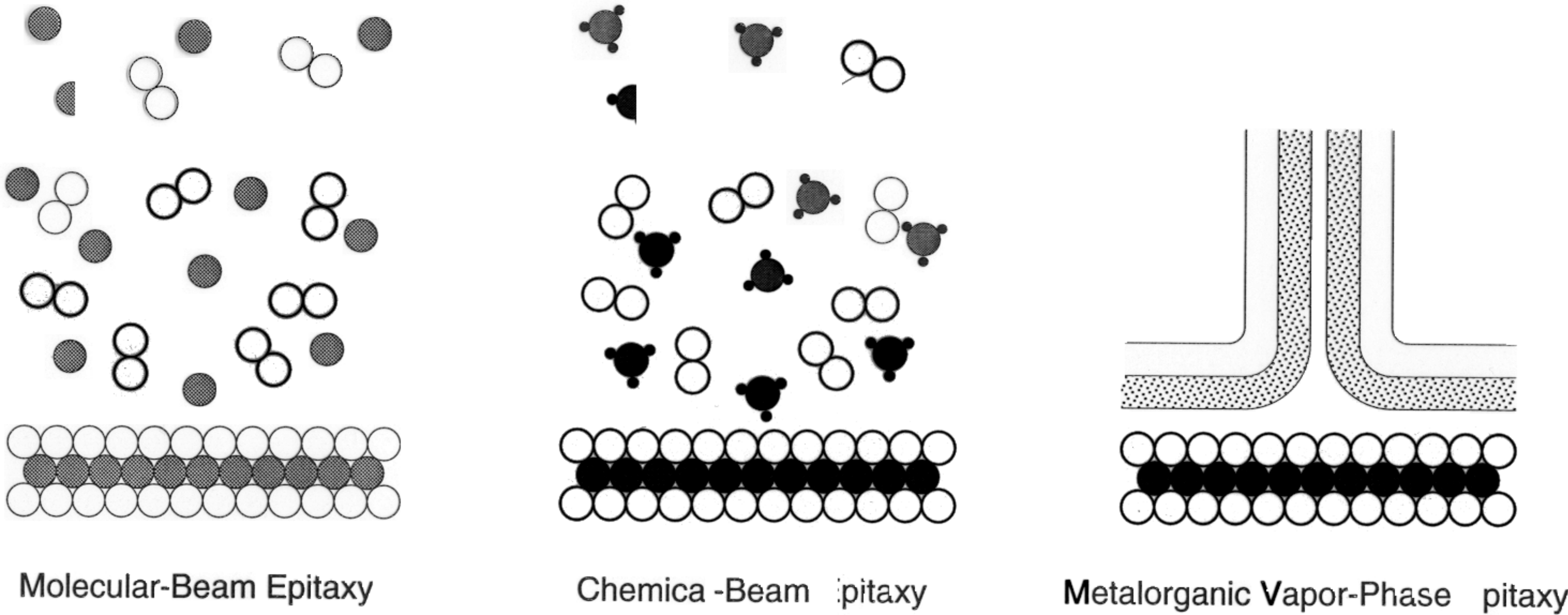
Island-size distributions

Multilayer Growth

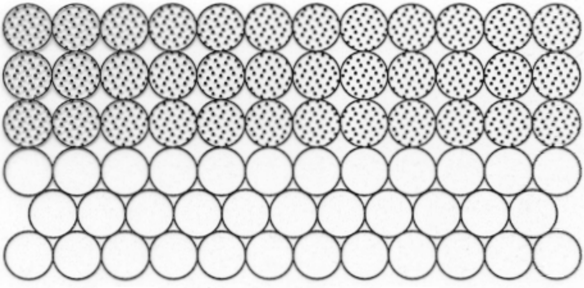
Kinetic roughening

Stranski Krastanov growth

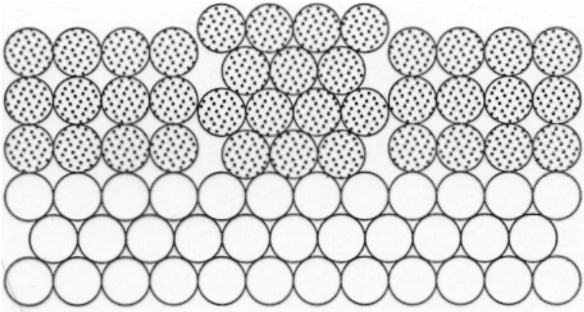
Summary



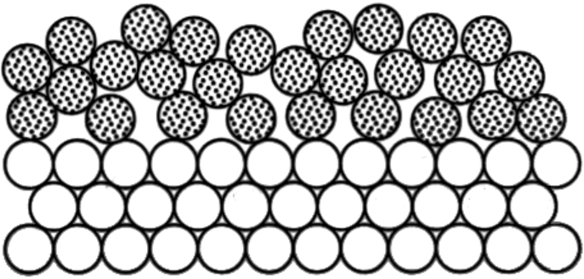
Molecular-Beam Epitaxy
Chemica -Beam :pitaxy
Metalorganic Vapor-Phase pitaxy



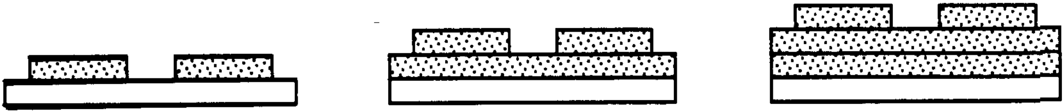
Epitaxial



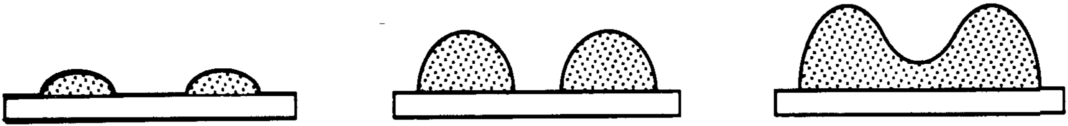
Polycrystalline



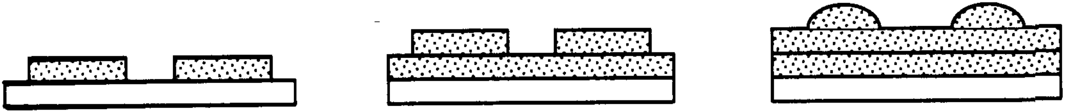
Amorphous



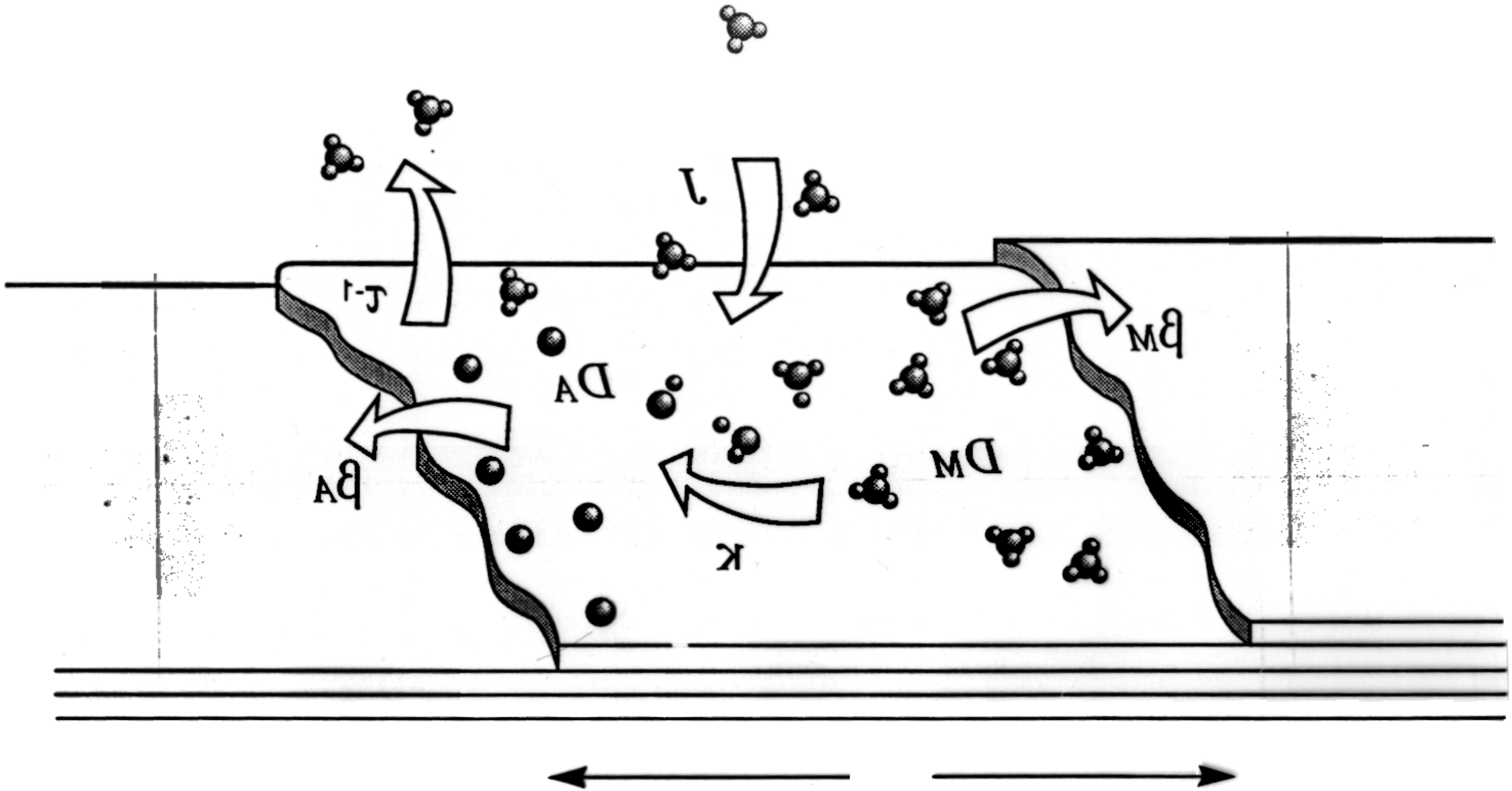
Frank-van der Merwe

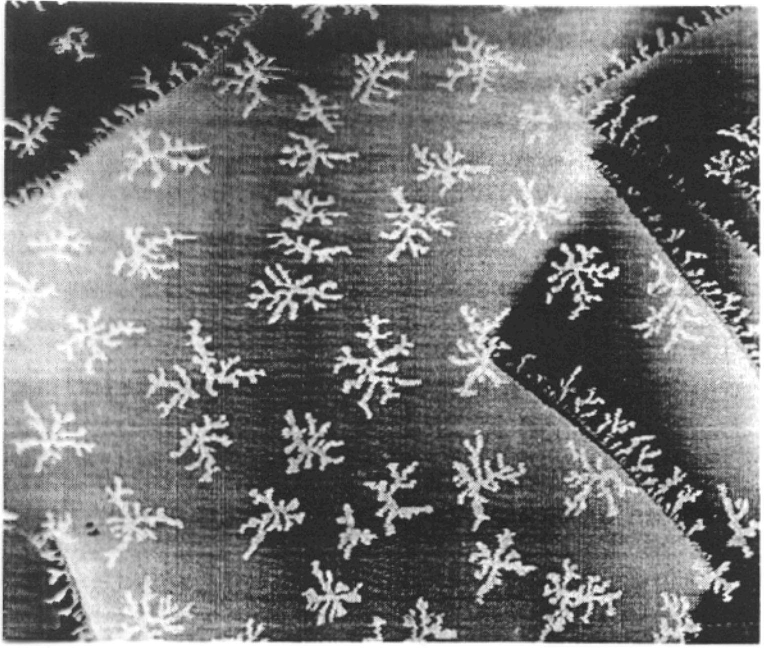


Volmer-Weber



Stranski-Krastanov

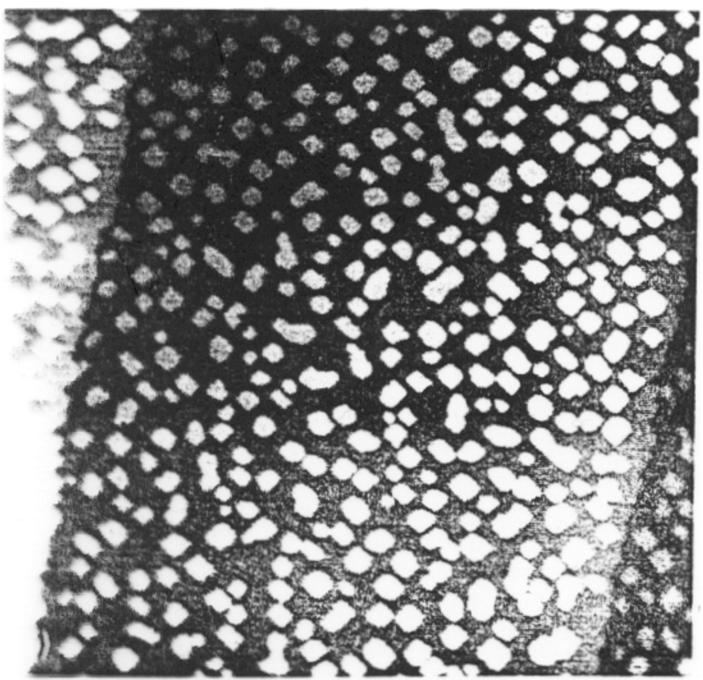

τ-1
J
DA
βA
κ
DM
βM



Au/Ru(0001)

$\beta \cong 1.7$

Phys. Rev. Lett. 67, 3279 ('91)



Ni/Ni(001)

$\beta \cong 2$

J. Vac. Sci. Technol. A 10, 1970 ('92)

Rate Equations

(Irreversible Aggregation)

$$\frac{dn_1}{dt} \quad F - 2D\sigma_1 n_1^2 \quad Dn_1 \sum_{s \; 2}^{\infty} \sigma_s n_s$$

$$\frac{dn_s}{dt} \quad Dn_1 \sigma_{s-1} n_{s-} \quad Dn_1 \sigma_s n_s$$

n_1 adatom density

n_s density of islands with s atoms

F deposition flux

D surface diffusion constant

σ_s. capture numbers

↑

contain spatial information about local environment

Scaling Laws

For large $R = D/F$, with $\theta = Ft$,

$n_1 \sim \theta^{-r} R^{-\omega}$ (adatom density)

$s_{av} \sim \theta^{z} R^{\chi}$ (average island size)

$N \sim \theta^{1-z} R^{-\chi}$ (total island density)

$n_s(\theta) = \dfrac{\theta}{s_{av}^2} f(s/s_{av})$ (individual island size)

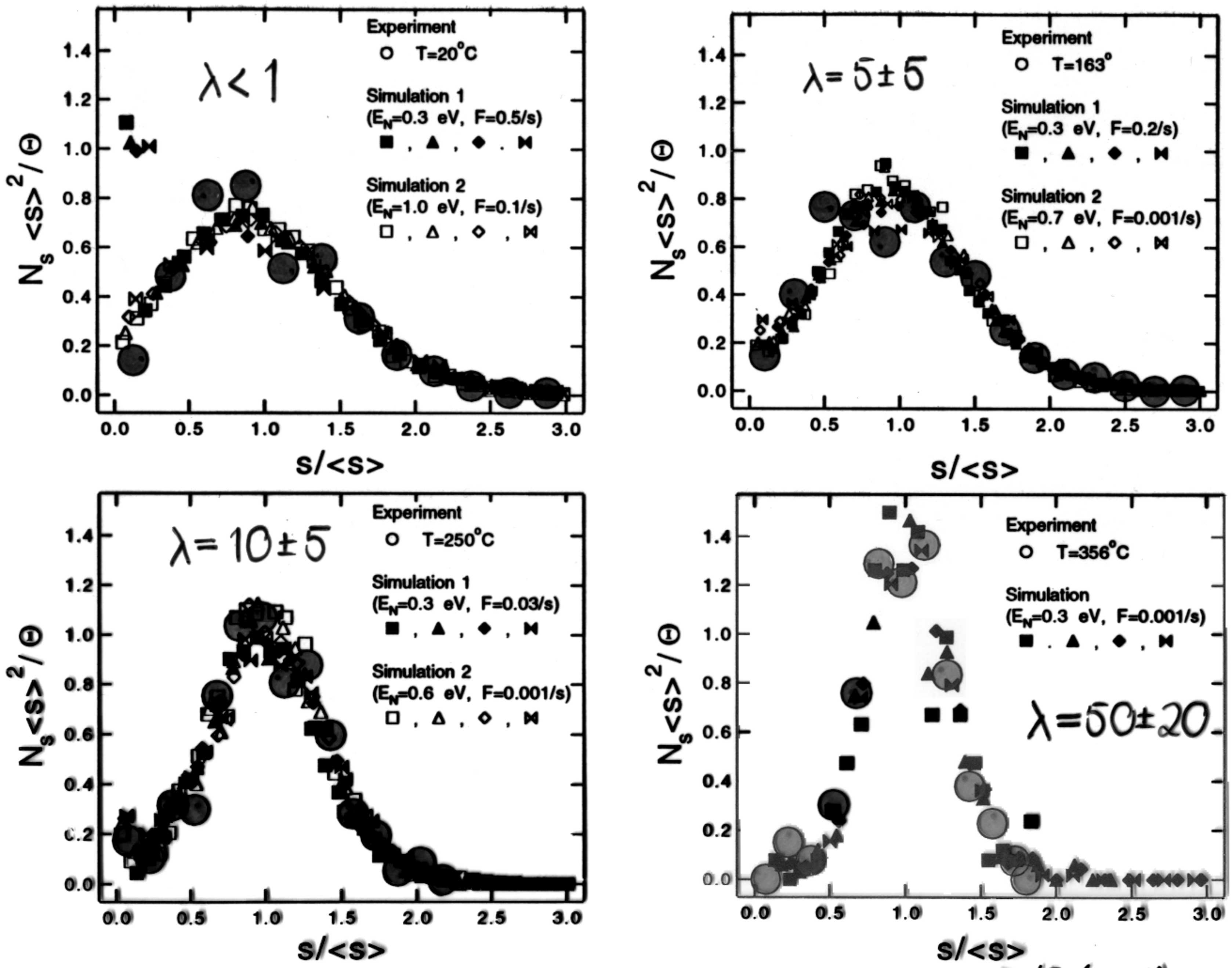
Exponents and scaling function are universal, but depend on processes:

detachment

evaporation

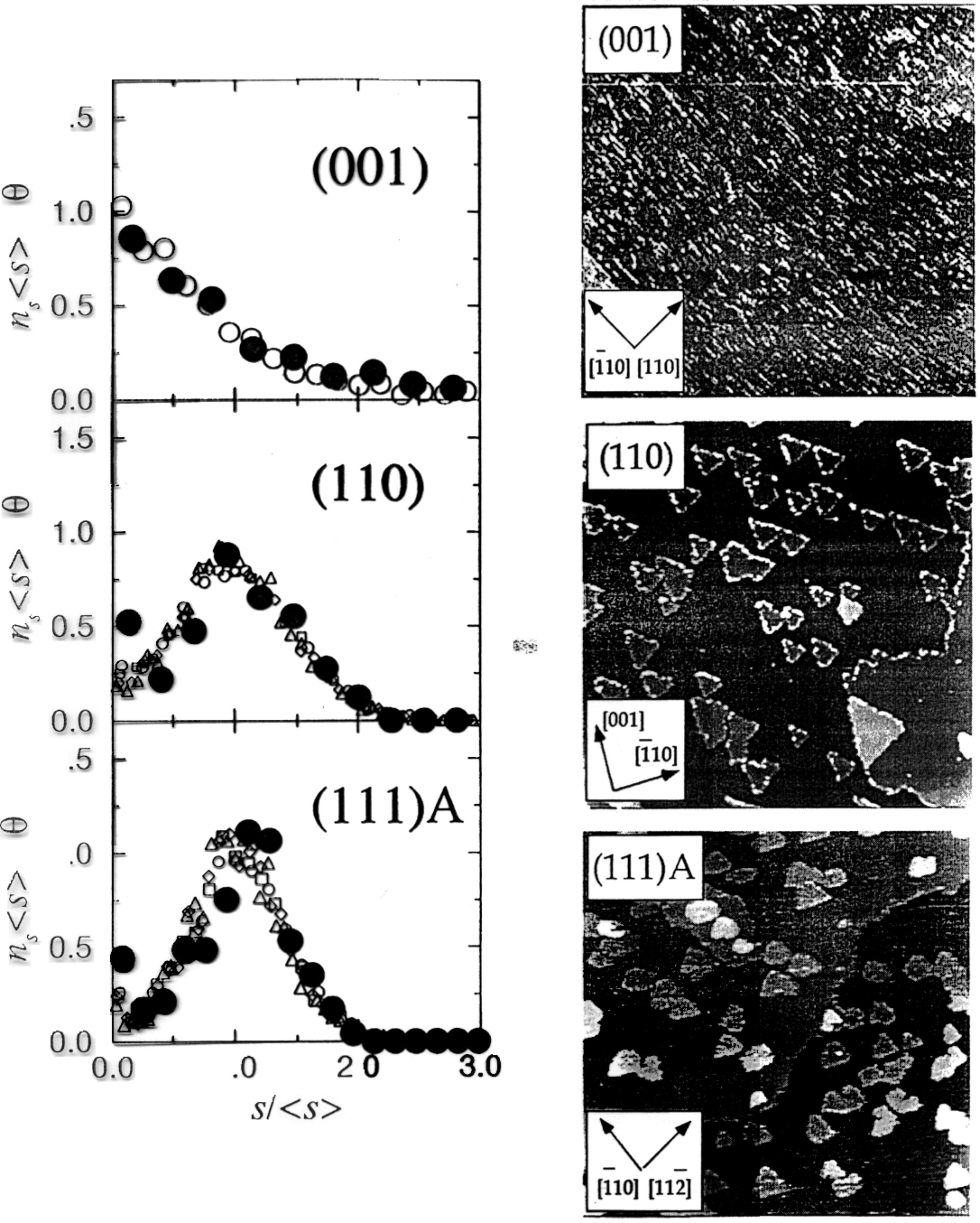
inhomogeneous nucleation

4. island mobility



$\lambda = N_1 e^{E_N/kT}$

Stroscio and Pierce, Phys. Rev. B. 49, 8522 (1994); STM on Fe/Fe(001)



(001)
(110)
(111)A
$n_s\langle s\rangle\ \theta$
$s/\langle s\rangle$
0.0
0.5
1.0
1.5
.5
.0
2.0
3.0
[$\bar{1}$10] [110]
[001]
[$\bar{1}$10]
[$\bar{1}$10] [11$\bar{2}$]

Island Dynamics (and Level Sets)

$$\frac{\partial n_1}{\partial t} \quad F + D\nabla^2 n_1 \quad 2\frac{dN}{dt}$$

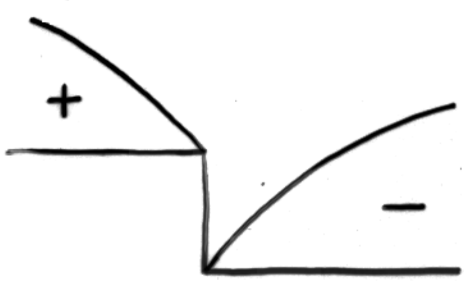
$$n_1(x \ t) \quad 0 \quad \text{for } \vec{x} \,\varepsilon\, \text{island boundary}$$

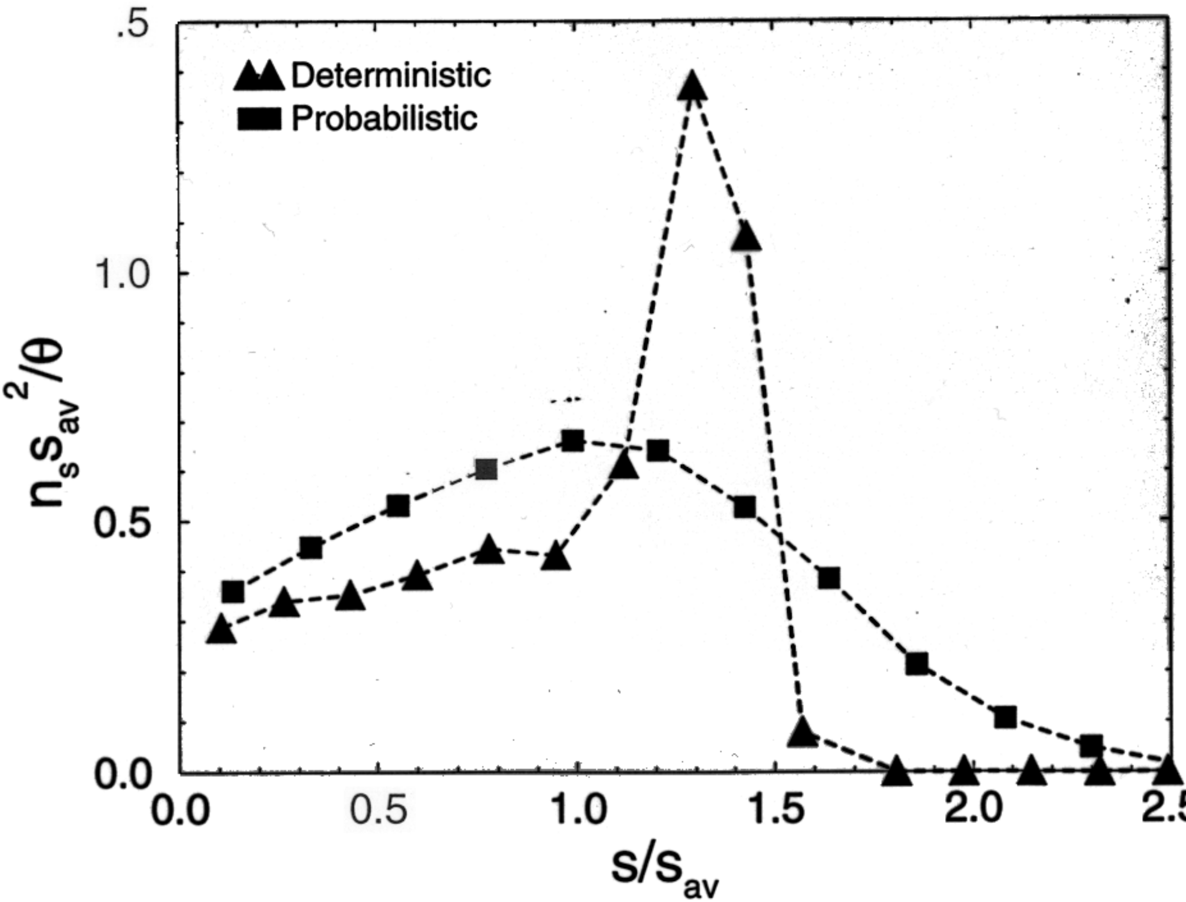
$$\frac{dN}{dt} \quad D\sigma \langle n_1^2 \rangle$$

Method of Solution

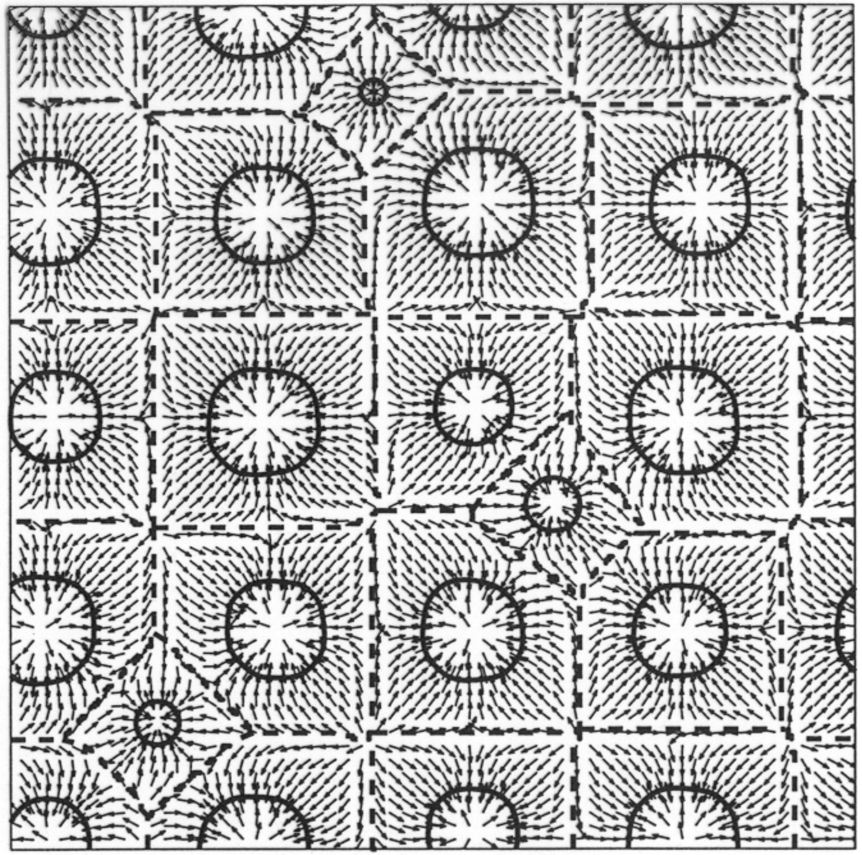
$$\frac{\partial \varphi}{\partial t} + v \ \nabla\varphi \quad 0$$

$$v_n \quad a^2 D\left(\hat{n} \ \vec{\nabla} n_1^- \quad \hat{n} \ \nabla n_1^+\right)$$

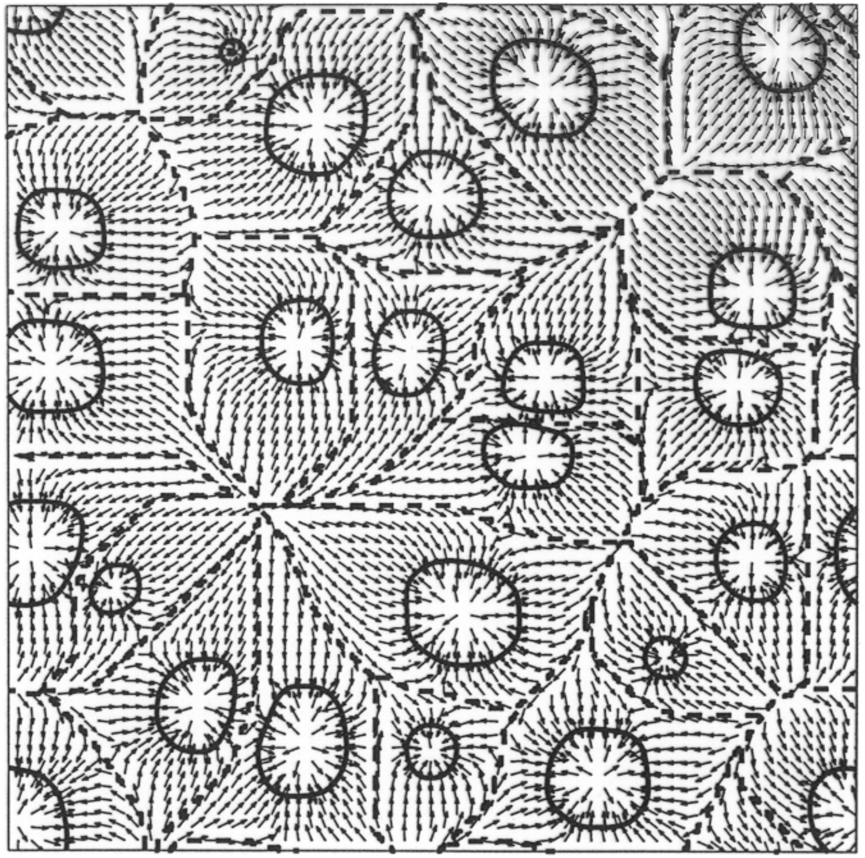




Deterministic
Probabilistic
.5
1.0
0.5
0.0
0.0
0.5
1.0
1.5
2.0
2.5
$n_s s_{av}^2/\theta$
s/s_{av}

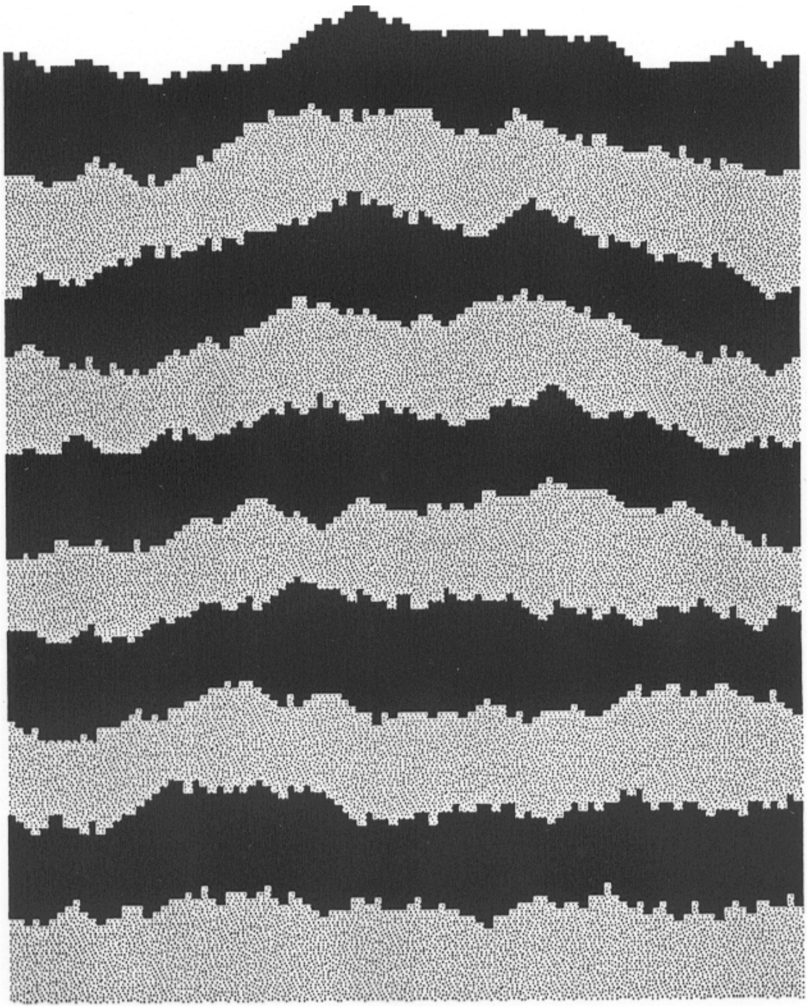


Deterministic Seeding



Stochastic Seeding

Kinetic Roughening



Random deposition + relaxation to local height minimum Edwards Wilkinson)

Barabási and Stanley Fractal Concepts in Surface Growth, p 45.

Kinetic Roughening

dynamic scaling hypothesis)

$$W(L\ t)\quad \{\langle h^2\rangle - \langle h\rangle^2\}^{1/2} \sim L^{\alpha} f(t/L^{z})$$

$h(\bar{x},t)$ surface height at position x at time t

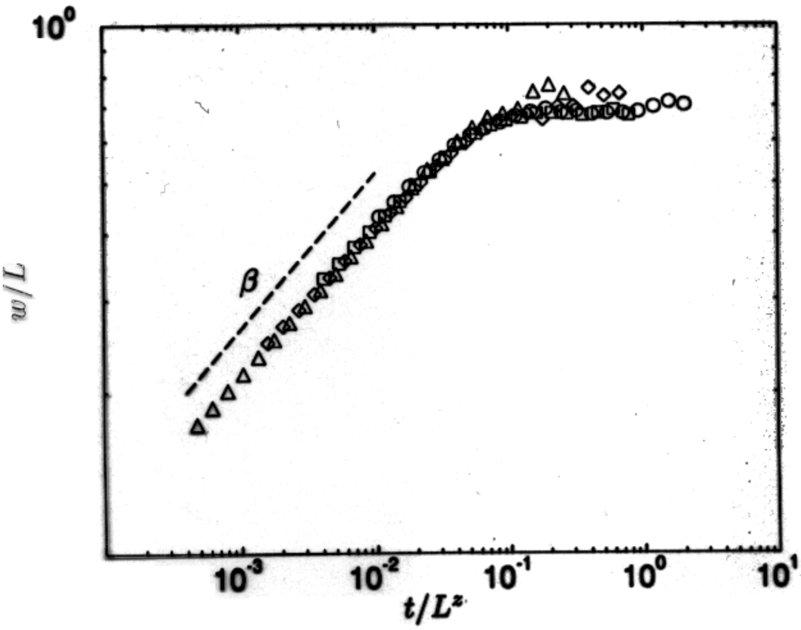
lateral viewing scale

$$\text{scaling function} \sim \begin{cases} x^{\beta}, & x \ll \\ \text{constant}, & x \gg \end{cases}$$

α roughess exponent

β growth exponent

$\Big\}\ z = \frac{\alpha}{\beta}$ dynamic exponent



Stochastic Equations of Motion

The problem to express discrete rule-based models as stochastic DEs

Such equations are expected to have the form

$$\frac{\partial h}{\partial t} \quad \gamma \nabla^2 h + \lambda (\nabla h)^2 + K \nabla^4 h + \sigma \nabla^2 (\nabla h \quad ^2$$

$$+ \quad + F + \eta$$

where

height of interface at position $\vec{x}$ at time t

Gaussian noise

Physical processes

γ: desorption EW relaxation

λ desorption

K, σ diffusion

F net flux

Passage across Length/Time Scales

Transition rules for atomistic lattice model KMC)

||

Master equation for $P(H, t)$ H $\{h_1, h_2, \quad \}$

↓

Kurtz theorems — van Kampen Ω-expansion

Discrete Fokker–Planck/Langevin equation

↓ ?

Continuum Equation of Motion

Summary

Three levels of scaling

fractal islands sland-size distributions,

kinetic roughening

Epitaxial phenomena

stochastic behavior + geometric motion

Multiscale modelling

atomistic processes → interface motion

Future work

development/application of analysis numerical

methods stochastic analysis/probability,...