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INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

SMR/917 - 9

SECOND WORKSHOP ON SCIENCE AND TECHNOLOGY OF THIN FILMS

(11 - 29 March 1996)

" Fractal/kinetic scaling treatment of film growth "

presented by:

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Surface Morphology and Kinetic Roughening of Ag/Ag(111)

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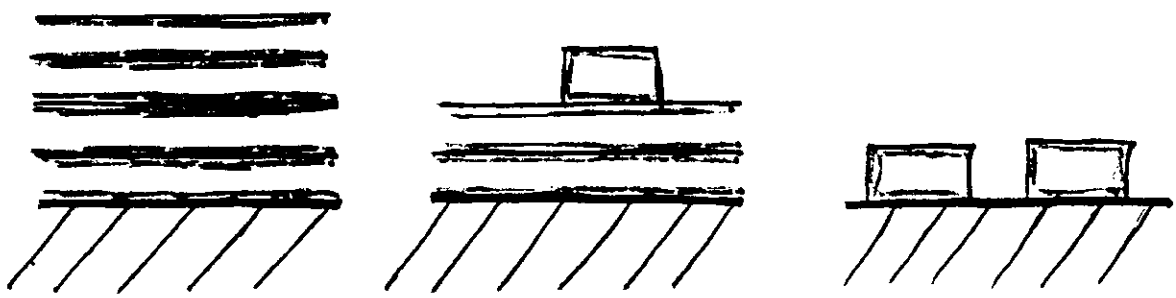


"Kinetic Roughening"

Family & Vicsek, 1985

$$\sigma(L,t) = L^H F(t/L^{H/\beta})$$

$$\sigma(L) \propto L^H \quad \text{for} \quad \frac{t}{L^{H/\beta}} \to \infty$$

$$\sigma(t) \propto t^\beta \quad \text{for} \quad \frac{t}{L^{H/\beta}} \to 0$$

"correlation length" $\xi \propto t^{1/z}$

$$z = H/\beta$$

for $R \gg \xi$ $\quad g(R) \to 2\sigma^2$

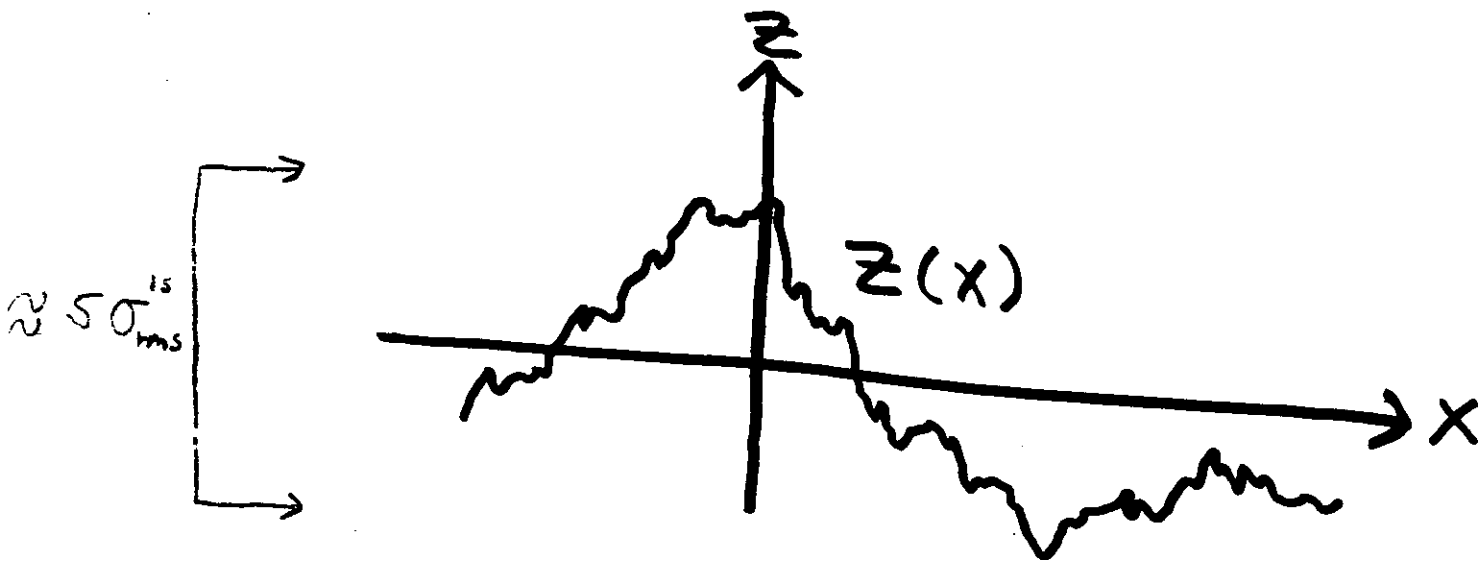
for $R \ll \xi$ $\quad g(R) = \langle [z(x',y') - z(x,y)]^2 \rangle$

$$g(R) \propto R^{2H} \qquad R = \sqrt{(y'-y)^2 + (x'-x)^2}$$

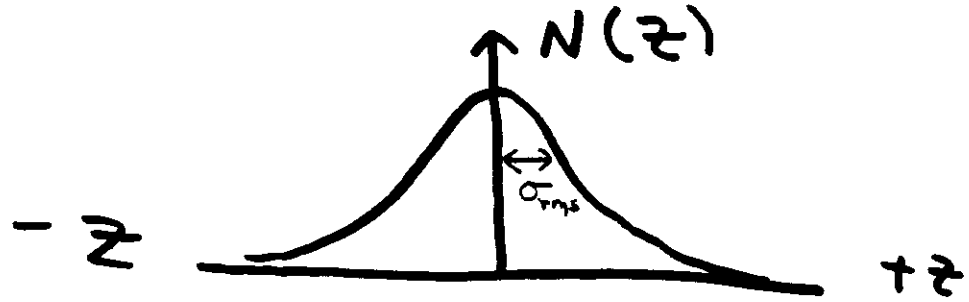
$C(R) = \langle z(R)\, z(0) \rangle = \sigma^2 - g(R)/2$

proposed form: $C(R) = \sigma^2 e^{-(R/\xi)^{2H}}$

Root-Mean-Square Roughness

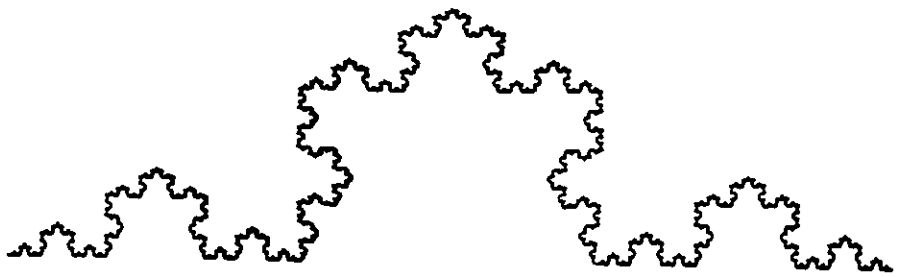


$$\sigma_{rms} = \sqrt{\langle z(x)^2 \rangle}$$

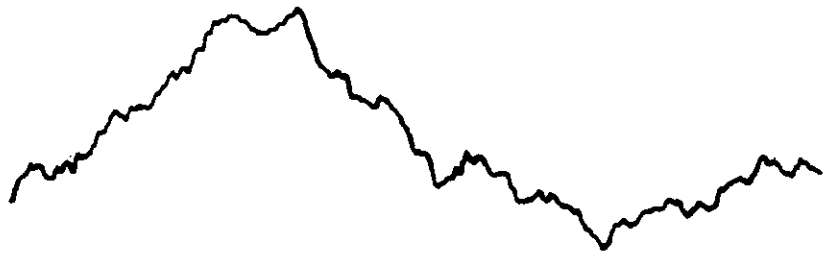


These surfaces have equal rms roughness.

Fractal scaling approach can further quantify the concept of roughness.



self-similar fractal

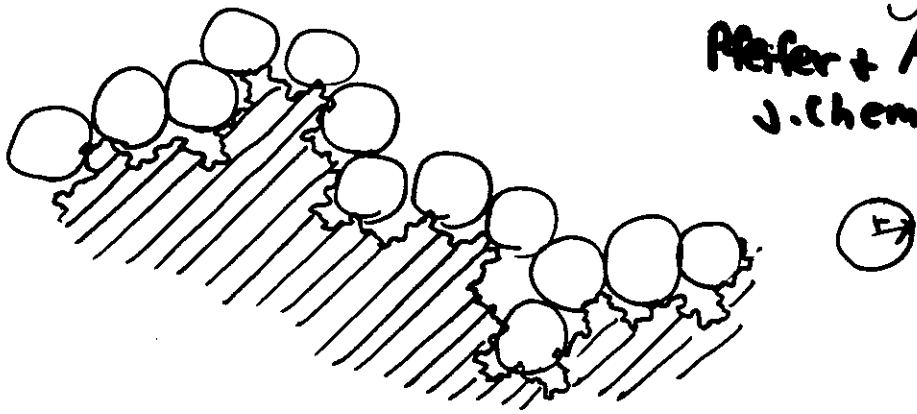


self-affine fractal

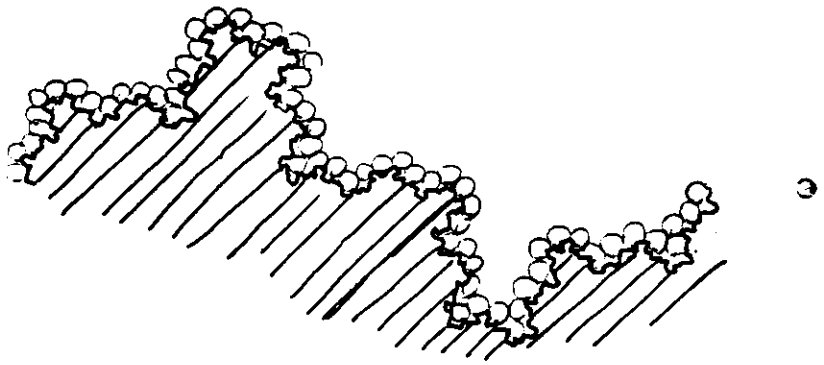
Figure 1

The fractal dimension

Can be probed with different sized coverings....



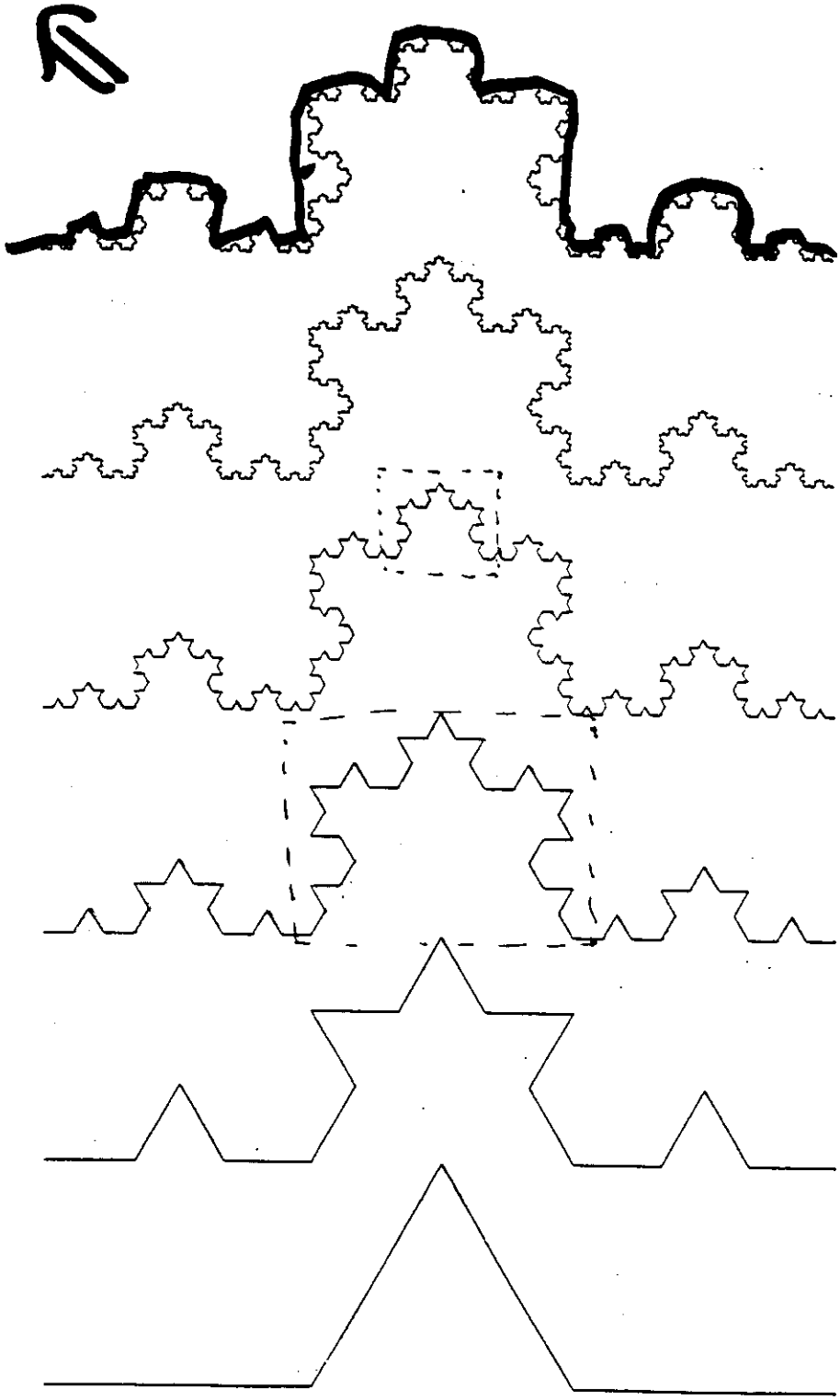
Pfeifer + Avnir
J. Chem Phys 1983



$$n \sim r^{-D}$$

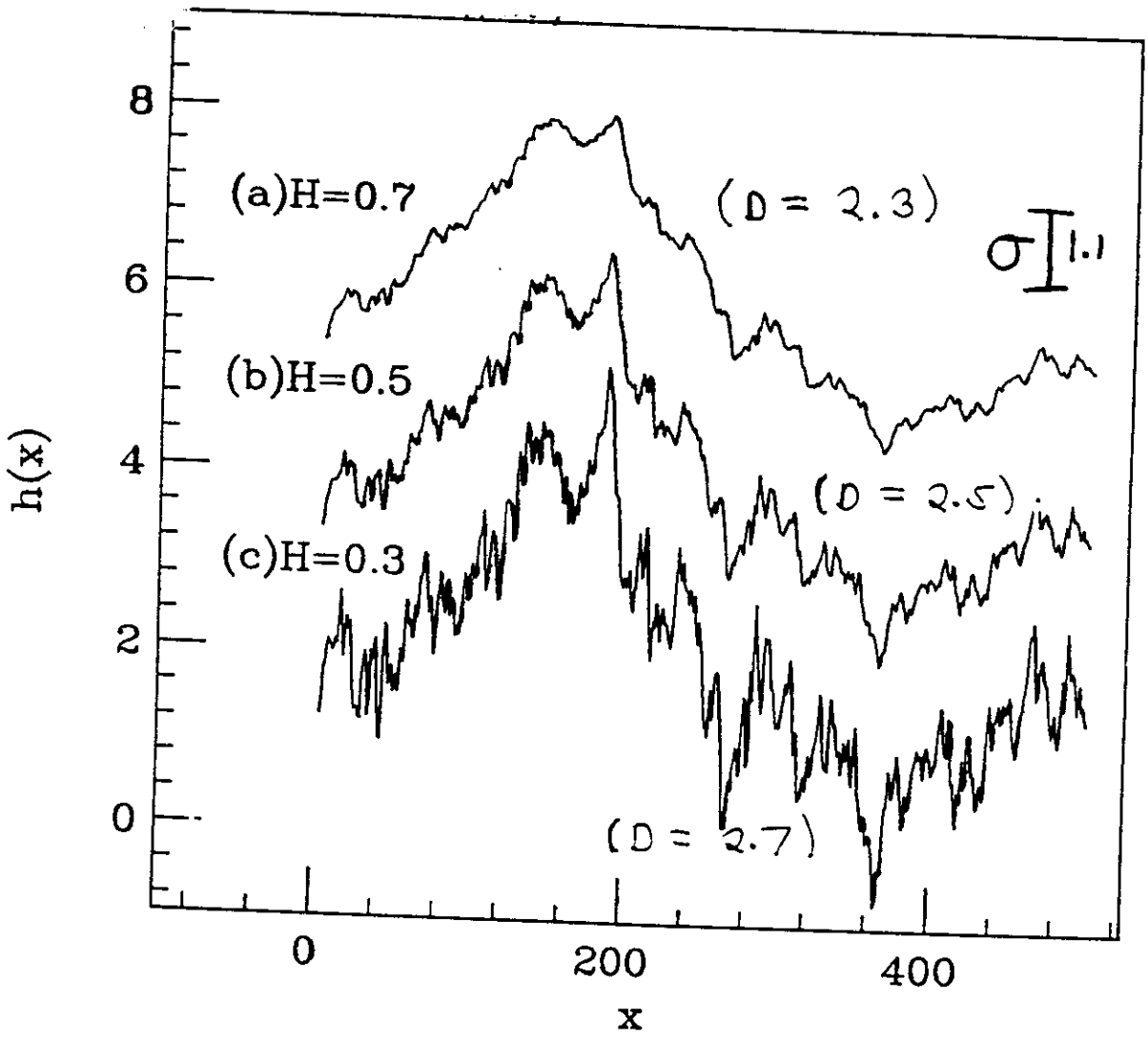
n: number of particles of radius r to cover the surface.

$D = H$



Self-Similar: Looks the same in its entirety as a portion of itself magnified...

$n \sim r^{-D}$ (n: number of radius r to cover surface)



Self-Affine Fractal Surfaces

$$h(bx) = b^{H} h(x) \quad ; \quad D = 3 - H$$

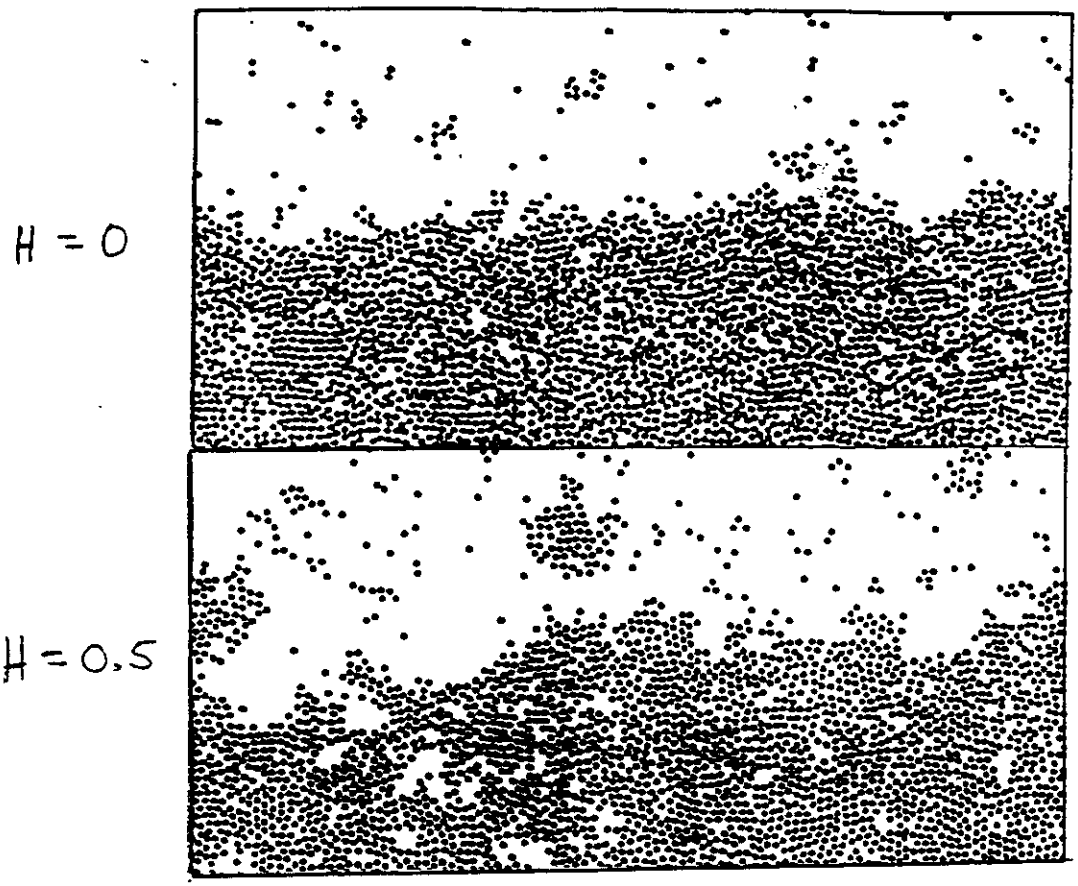
root-mean-square "roughness"

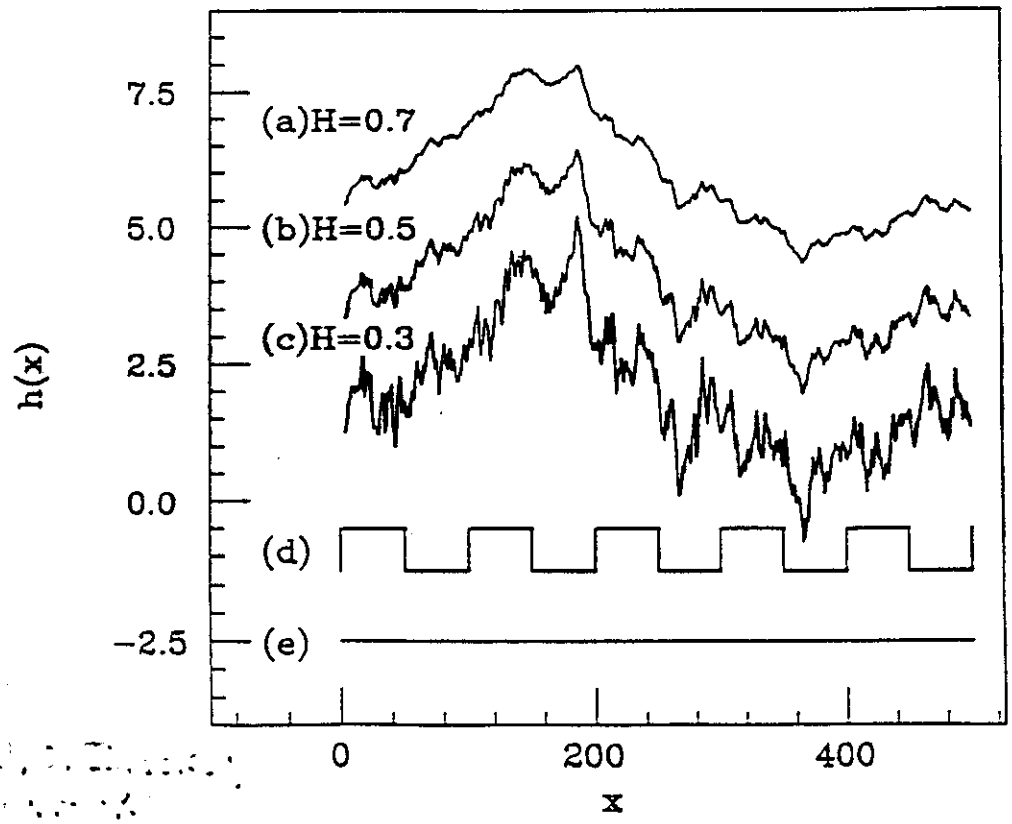
$$\sigma = \sqrt{\langle (h(x) - \bar{h}(x))^2 \rangle}$$

$$\sigma \sim L^{H}$$

L: scan size

("H" is commonly called "α")


H = 0
H = 0.5


7.5
5.0
2.5
0.0
−2.5
h(x)
(a)H=0.7
(b)H=0.5
(c)H=0.3
(d)
(e)
0
200
400
x

Barabasi & Stanley
"Fractal Concepts in Surface Growth"

contact properties, avoiding as much as possible the roughening process. However, in many cases roughening cannot be avoided, even in materials with promising technological potential. Understanding the roughening process might help map the experimental and technological limits, hopefully leading to the discovery of methods to control the interface roughness.

Motivated by the advances in modeling and predicting the roughening processes, a number of experimental groups recently have turned their attention to checking the theoretical predictions. In Chapter 16 we describe some experiments that confront theoretical results with the reality of the laboratory.

12.2 Microscopic processes on crystal surfaces

Before beginning a detailed study of the possible growth equations describing the growth of crystal interfaces by atom deposition , we review the relevant microscopic processes taking place on the crystal interface (see Fig. 12.1). The morphology of the interface is determined by the interplay between *deposition*, *desorption*, and *surface diffusion*.

12.2.1 Deposition

An atom from the vapor arrives at a random position on the interface, forms bonds with the surface atoms, and sticks. This process is termed *deposition* (see Fig. 12.1). Crystals grow by atomic deposition:

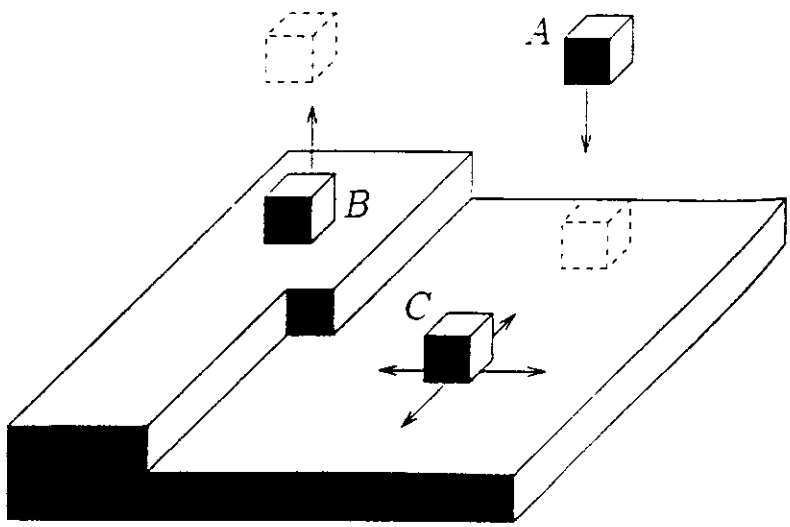


Figure 12.1 Elementary processes on a crystal surface. (*A*) Atoms arrive on the surface, where they are deposited. (*B*) An atom on the surface may *desorb*, leaving the surface of the crystal. (*C*) Atoms *diffuse* in random directions on the surface.

edge of the island, increasing the number of neighbors. This process results in more compact clusters.

This transition is illustrated in Fig. 17.3, where not the temperature but rather E_N is varied. The result is similar to changing the temperature. If E_N is large, the attachment to the island of a diffusing atom is almost irreversible, and the islands have a fractal structure. However, decreasing E_N increases the probability of an atom detaching from the island or diffusing along the island perimeter. Hence, the islands become non-fractal, acquiring a compact shape. While this model is quite different from the DDA model, especially in the small E_N region, it does show scaling properties that are similar to those of the DDA model. In particular the scaling law (17.4) is obeyed for a range of

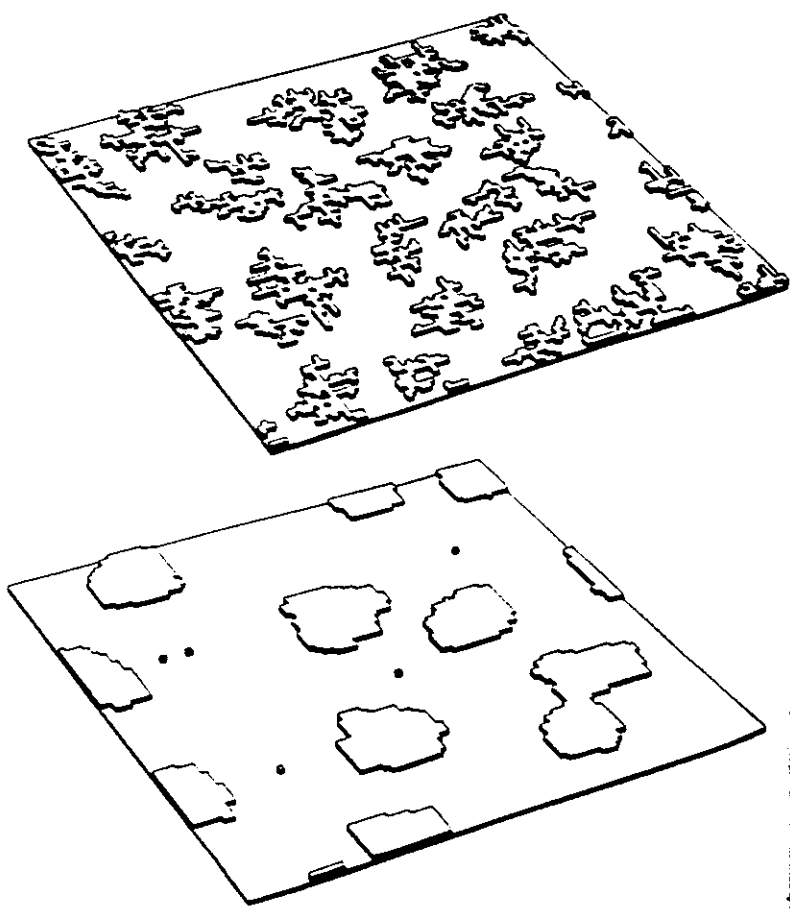


Figure 17.3 Typical island morphology at coverage $\Theta = 0.2$ for a 100×100 section of a 400×400 system obtained using Monte Carlo simulations with activated diffusion. For the top panel $E_N = 1.0$ eV, while for the bottom panel $E_N = 0.3$ eV. Note the transition from fractal to compact clusters as the bond energy decreases. (After [378]).

C. Ratsch et al. PRL 72, 3194 (1994)

Continuum Models of Nonequilibrium Growth

Rate of change of the film height h: $\frac{\delta h(x,t)}{\delta t} =$

Average deposition rate: R_d (1)

"Noise": fluctuations in the deposition rate: $+\eta(x,t)$ (2)

$+\nu\nabla^2 h$ "Surface tension": smooths out bumps (3)

Non linear term": slope-dependent growth rate; does not conserve mass: $+\frac{\lambda}{2}(\nabla h)^2$ (4)

$-\kappa(\nabla^4 h)$ "Partial", or "modified" smoothing: partial falls.... (5)

"Modified" smoothing: high to low steps: $+\sigma\nabla^2[\nabla h]^2$ (6)

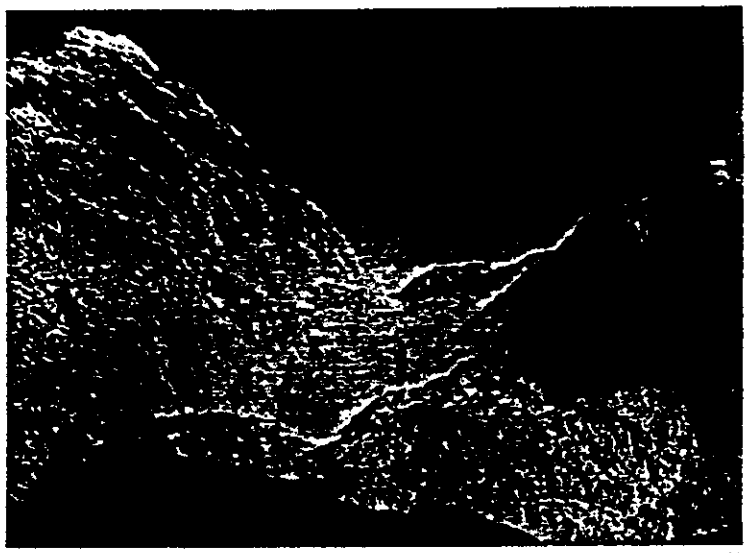
+..... "full" diffusion ... (just include everything) (7)

MODEL	H	β	z
KPZ (1,2,3,4)	≈ 0.35	0.25	≈ 1.4
"pure diffusion" (1,2,5)	1	0.25	4
Edwards-Wilkinsen (1,2,3[redacted])	0	0	2
MBE (1,2,5,6)	0.67	0.20	10/3
"full diffusion" (1,2,3,5,6,7)	0.4 - 1	0.25-1	

Kardar, Parisi, Zhang, PRL 56, 889 (1986); Edwards-Wilkinsen P.R.S. London A381 17 (1982)
Villain, J. Phys. I (Paris) (1991); Wolf & Villain Europhysics Lett 13, 389 (1990)
Lai & Das Sarma PRL 66, 2348 (1991) - - - - - - -

D = 2.15

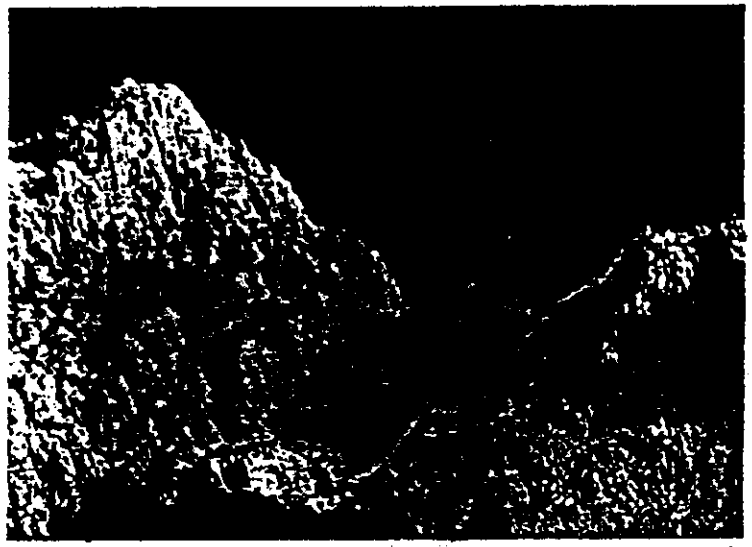
H = .85



← L + d.S. "MBE"

D = 2.5

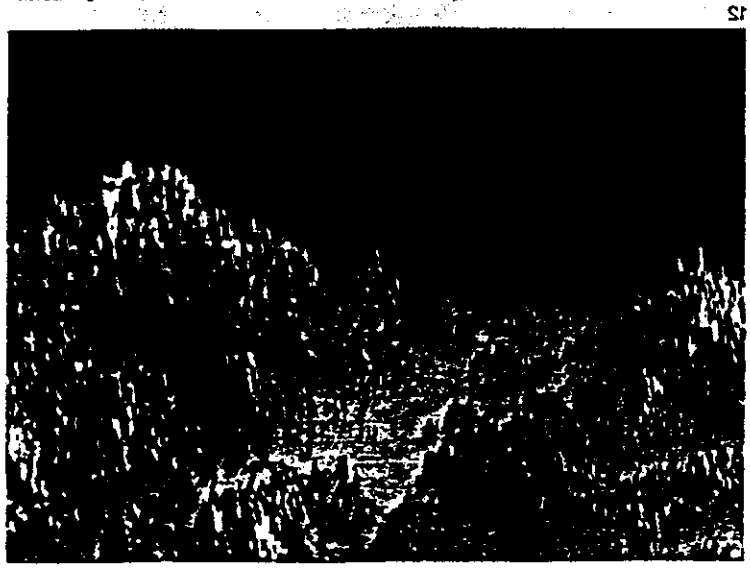
H = .5



← KPZ

D = 2.8

H = .2



R. Voss, in "The Science of Fractal Images"

With some algebra [340] we find, after the inverse transform back to real space, the result

$$\langle h(\mathbf{x},t)h(\mathbf{x}',t')\rangle = \frac{D}{2\nu}\,|\mathbf{x}-\mathbf{x}'|^{2-d}\; f\left(\frac{\nu\,|t-t'|}{|\mathbf{x}-\mathbf{x}'|^{z}}\right). \tag{5.21}$$

Here $f(u)$ is a scaling function with the properties $f(u) \to$ const as $u \to \infty$ and $f(u) \to u^{(2-d)/z}$ as $u \to 0$. Comparing (5.21) with (2.8), we obtain the same scaling exponents (5.16).

For $d = 2$, we find $\alpha = \beta = 0$, confirming the scaling result (5.16). In this case the correlations decay logarithmically, i.e., the width scales logarithmically with time at early times, and the saturation width depends on the logarithm of the system size. We find $t_\times \sim L^z$ so $z = 2$, confirming (5.16).

For the EW equation, we find that the scaling exponents depend on

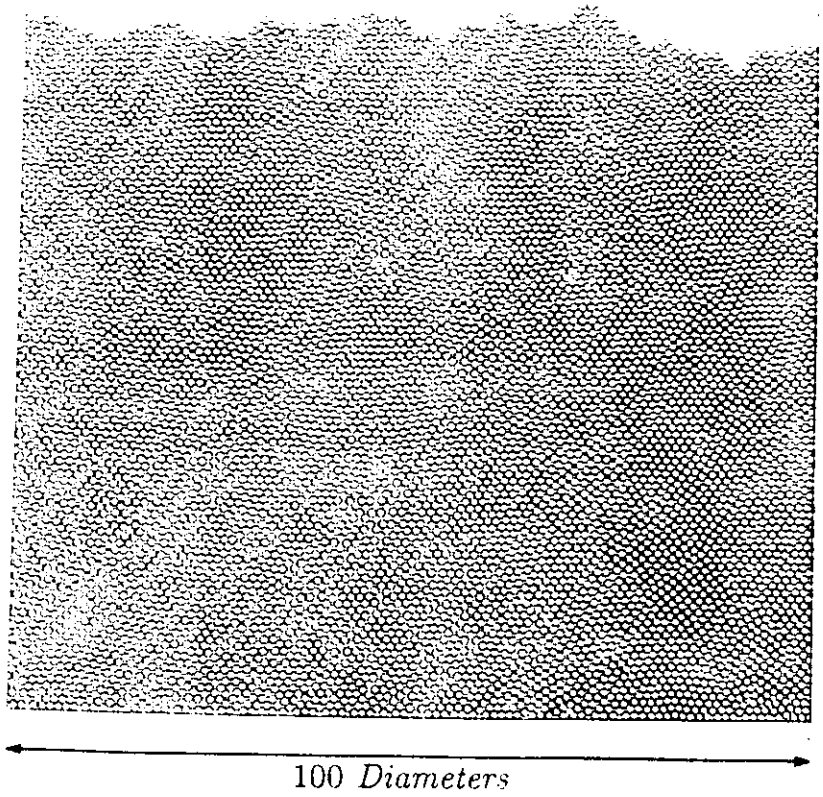
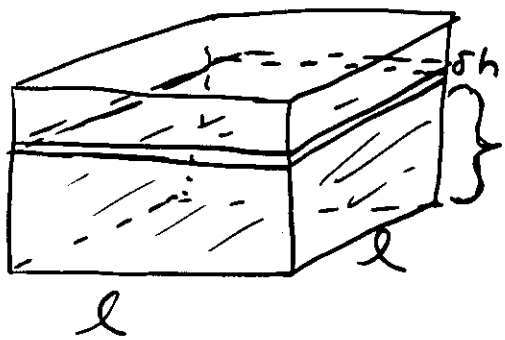


Figure 5.5 *Off-lattice* random deposition with surface relaxation. (After [307]).

Let ℓ be the average distance a Ag atom moves before being incorporated. (distance between steps??)



what is δh? (i.e. σ)

N atoms to fill the box to height h. The uncertainty in N (due to beam fluctuations) is $\sqrt{N}$

which will result in a height "uncertainty" (width) $\sigma = \frac{\sqrt{h}}{\ell}$

Including surface tension: $\sigma \leftarrow \frac{\sqrt{h}}{\ell}$ (if all is well with the model)

The horizontal scaling behavior provides us with an independent estimate of ℓ....

$$\sigma(L) = A' \left(\frac{L}{\ell}\right)^{2/3}$$

At $h = 253$, $\sigma(h{=}1000) = 9.2$ (from data)

Assume $\sigma(L = \ell) = (.2 \to 1)$ (i.e one step with height 1)

$$\Rightarrow A' \cong .2$$

$$\Rightarrow 9.2 = (.2 \to 1)\left(\frac{1000}{\ell}\right)^{2/3}$$

$$\Rightarrow \boxed{\ell \approx 3\text{-}30}$$

largely consistent with $\sigma(\ell) < \frac{\sqrt{h}}{\ell}$

Lecture II Conclusion:

The concept of kinetic roughening provides a framework for quantitative analysis of non-equilibrium film growth.

Does it reveal anything about the physical processes underlying growth??