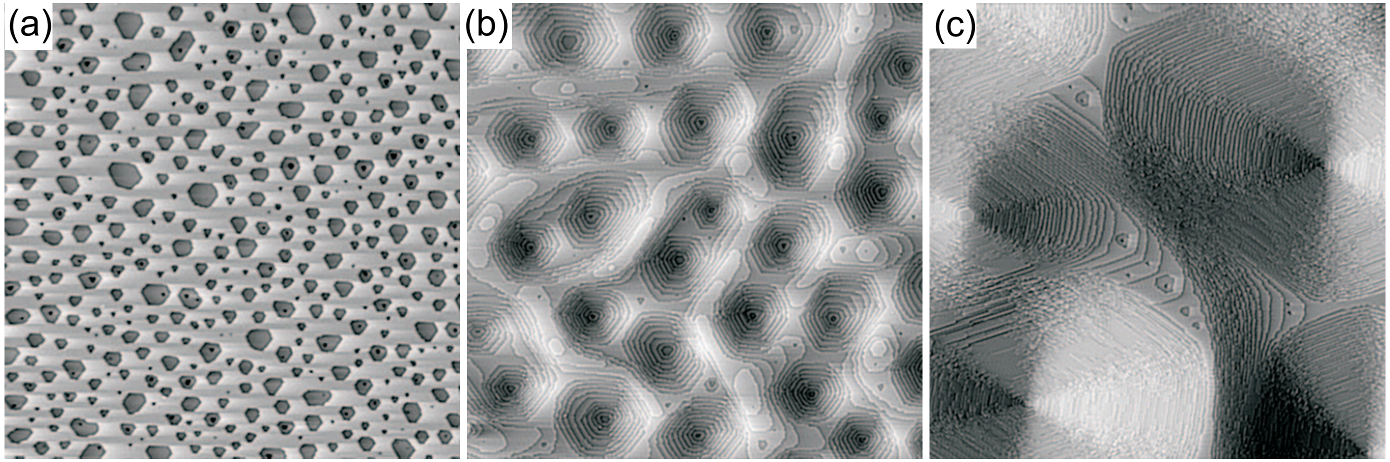
Scaling Concepts in Surface Science



Ion erosion of Pt(111) (T. Michely)

"How, precisely, can one confront theory with reality? Without this crucial step, there can be no science." Per Bak

Symposium COMPLEXITY AND CRITICALITY in memory of Per Bak
Niels Bohr Institute, Copenhagen, August 21-23 2003

Empirical science is apt to cloud the sight, and, by the very knowledge of functions and processes, to bereave the student of the manly comtemplation of the whole. The savant becomes unpoetic. But the best read naturalist who lends an entire and devout attention to the truth, will see that there remains much to learn of his relation to the world, and that it is not to be learned by any addition or subtraction or other comparison of known quantities, but is arrived at by untaught sallies of the spirit, by a continual self-recovery, and by entire humility.

He will perceive that there are far more excellent qualities in the student than preciseness and infallibility; that a guess is often more fruitful than an indisputable affirmation, and that a dream may let us deeper into the secret of nature than a hundred concerted experiments.

Ralph Waldo Emerson, *Nature* (1836)

Why power laws ?

- because they are simple
  absence of a characteristic scale, independence of microscopic details

- because they are beautiful
  self-similarity, scale invariance

- because they are useful
  universality classes, zoology of scaling exponents

- because they provide **regularities** in the description of **irregular** phenomena

Is the power law

the signal

or

the noise?

Trivial vs. nontrivial power laws

- **trivial**: free fall $x \sim t^2$
  diffusion, central limit theorem $\langle x^2 \rangle \sim t$
  mean field theory
  dimensional analysis ? K41 ?
  linear theories ?? persistence ??
  $1/f$-noise from defect trapping

- **nontrivial**: Onsager exponents
  diffusion-limited aggregation $D_{\mathrm{DLA}} \approx 1.71...$
  kinetic roughening $\beta_{\mathrm{KPZ}} \approx 1/(d+2)$
  intermittency corrections in turbulence
  .....

Scaling in surface physics: Some milestones

- size-dependent time scales in coarsening, sintering & smoothing [Herring, Mullins, Lifshitz-Slyozov-Wagner...]
- self-affine surfaces in fracture & geomorphology [Mandelbrot, Voss,...]
- kinetic roughening of growing surfaces $\sigma = \sqrt{\langle (h - \overline{h})^2 \rangle} \sim (\overline{h})^{\beta}$ [Plischke & Rácz, Family & Vicsek, Kardar-Parisi-Zhang, Villain,....]
- scaling of island size distributions [Bartelt & Evans, Amar & Family, Mulheran & Blackman,...]

Issues:

- How are scaling concepts used in surface science?
- Have nontrivial exponents been found?

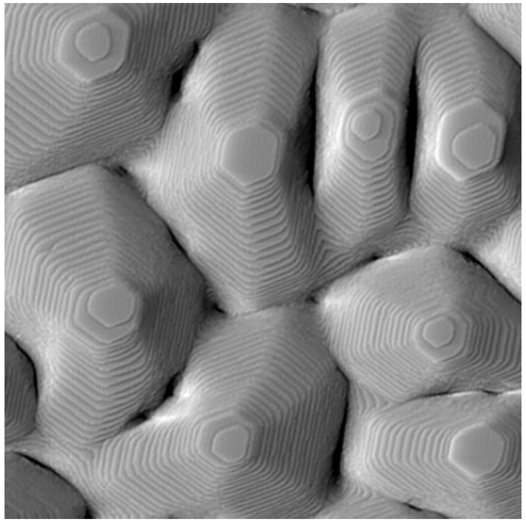
Mechanisms for surface roughening

Stochastic roughening:

- competition between smoothing and random noise
- self-affine morphology with nontrivial exponents
- $\beta < \beta_{\mathrm{Random\ Deposition}} = 1/2$

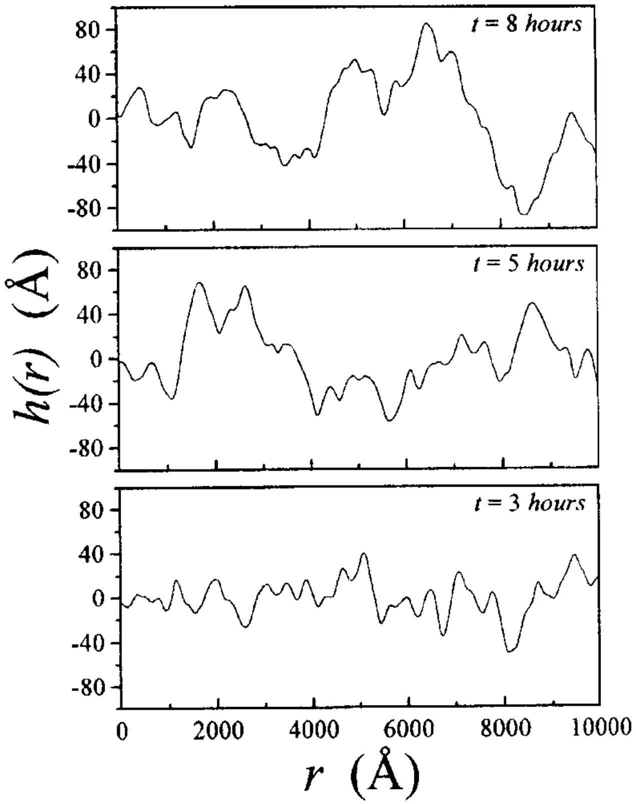
Mound formation:

- deterministic instability of the flat surface
- characteristic length scale & coarsening $\Rightarrow$
- known models yield $\beta = 1/3$ or $1/2$



Roughening of amorphous silicon

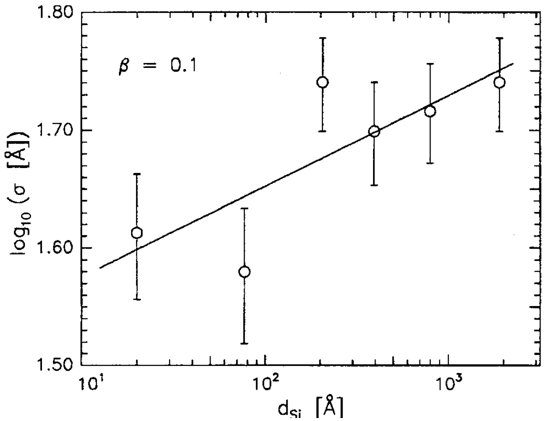
- Real space view:

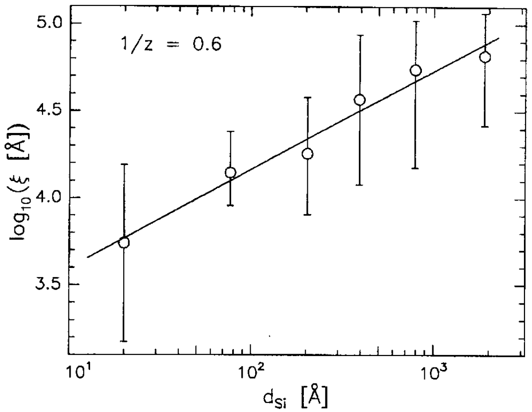


$\Rightarrow$ noisy Mullins ($\beta = 1/4$)

Yang et al., PRL 76, 3774 (1996)

- Scaling laws:





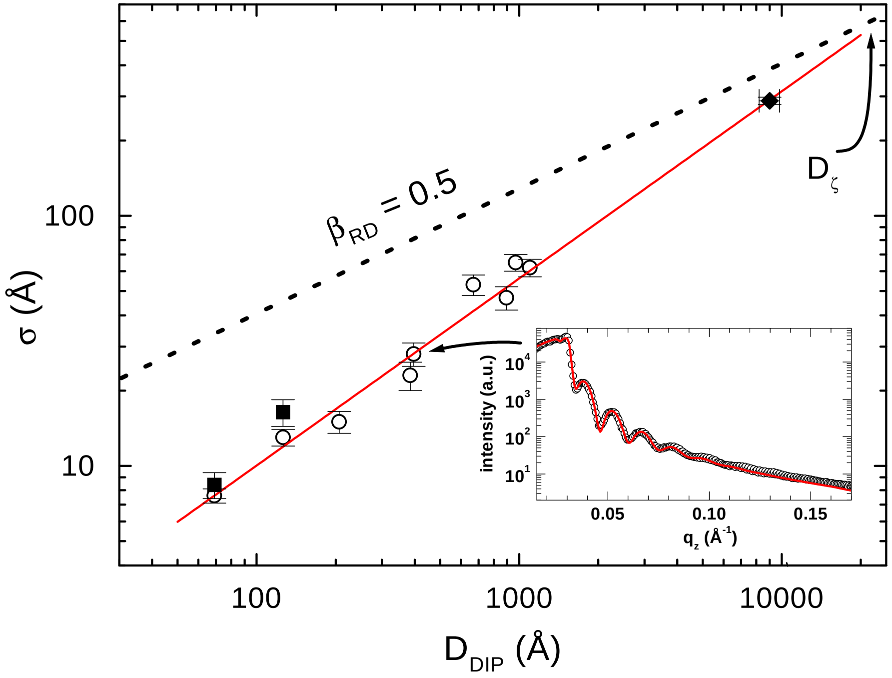
$\Rightarrow$ KPZ behavior ($\beta \approx 0.1$)

Lütt et al., PRB 56, 4085 (1997)

Roughening of organic thin films

[A.C. Dürr et al., PRL 90, 016104 (2003)]

Rapid roughening: $\beta > \beta_{\text{Random Deposition}} = 1/2$ here: $\beta \approx 0.75$

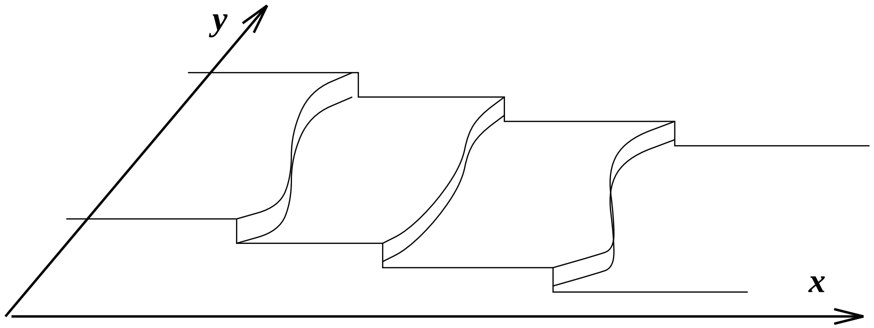


- Is it possible that also $\sigma > \sigma_{\text{RD}} = d\sqrt{h/d}$?

- Hypothesis:
  Tilt-domains lead to phase-disordered KPZ behavior
  $\Rightarrow \quad \sigma \sim t/\ln(t)^{\psi}$

Scaling of step fluctuations

- Steps on a vicinal crystal surface are thermally rough one-dimensional manifolds



- static scaling: $\langle |x(y) - x(y')|^2 \rangle = (k_\mathrm{B} T/\tilde{\delta}) |y - y'|$ $\tilde{\delta}$: step stiffness

- kinetic universality classes: [N.C. Bartelt, T.L. Einstein, E.D. Williams,...]

$$\frac{\partial}{\partial t} x(y,t) = -A \left(-\frac{\partial^2}{\partial y^2} \right)^{z/2} x(y,t) + \text{noise}$$

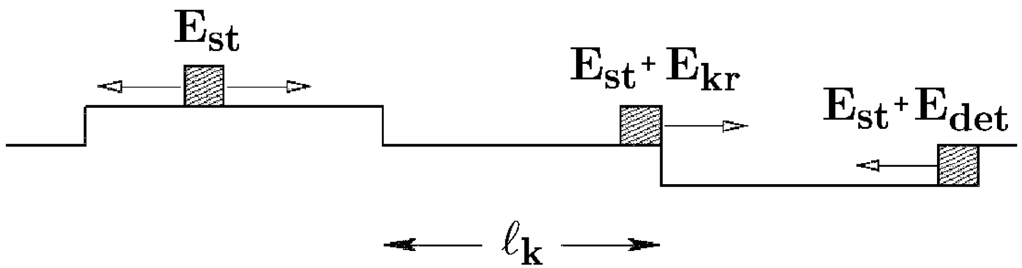
$z = 2$: attachment-detachment kinetics $\Rightarrow$ $\langle x^2 \rangle \sim t^{1/2}$, $\beta = 1/2z = 1/4$
$z = 4$: edge diffusion $\Rightarrow$ $\langle x^2 \rangle \sim t^{1/4}$, $\beta = 1/8$
$z = 3$: terrace diffusion $\Rightarrow$ $\langle x^2 \rangle \sim t^{1/3}$, $\beta = 1/6$

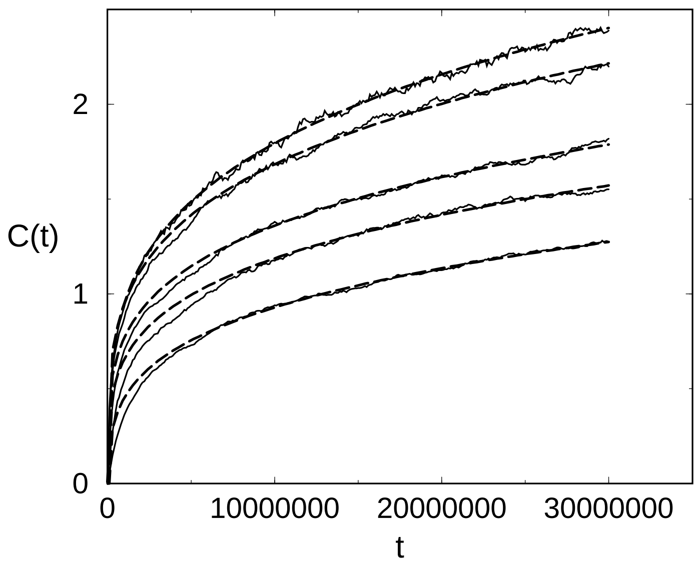
Step fluctuations and kink rounding barriers

[J. Kallunki, J.K., Surf. Sci. Lett. 523, L53 (2003)]

Microscopic processes
at the step edge:

- edge diffusion $E_{\rm st}$
- kink detachment $E_{\rm det}$
- **kink rounding** $E_{\rm kr}$





$\Rightarrow C(t) = \langle [x(y,t) - x(y,0)]^2 \rangle = Bt^{1/4}$

with $B \sim \exp[-E_a/k_{\rm B}T]$

$$E_a = \begin{cases} (E_{\rm st} + 5\varepsilon)/4 & E_{\rm kr} < \varepsilon \\ (E_{\rm st} + E_{\rm kr} + 4\varepsilon)/4 & E_{\rm kr} > \varepsilon \end{cases}$$

ε: kink energy

Application to Cu(100): $E_{\rm kr} \approx 0.41$ eV

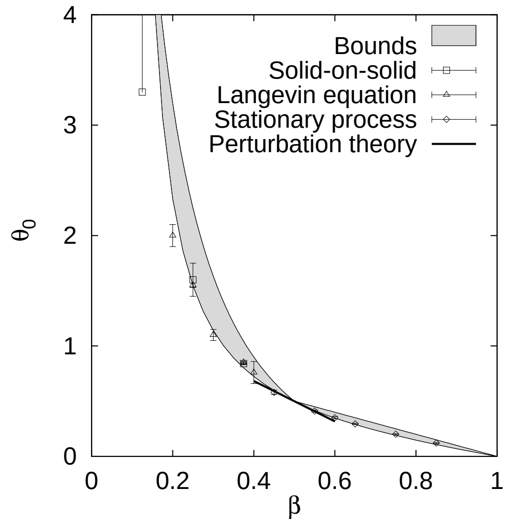
Persistence of step fluctuations

Persistence probability: [PRE 56, 2702 (1997)]

$$P(t_0, t) \equiv \mathrm{Prob}[x(s) \neq x(t_0) | t_0 \leq s \leq t_0 + t]$$

$$P(t_0 \gg t) \sim t^{-\theta_S}, \quad \theta_S = 1 - \beta \qquad \text{“trivial”}$$

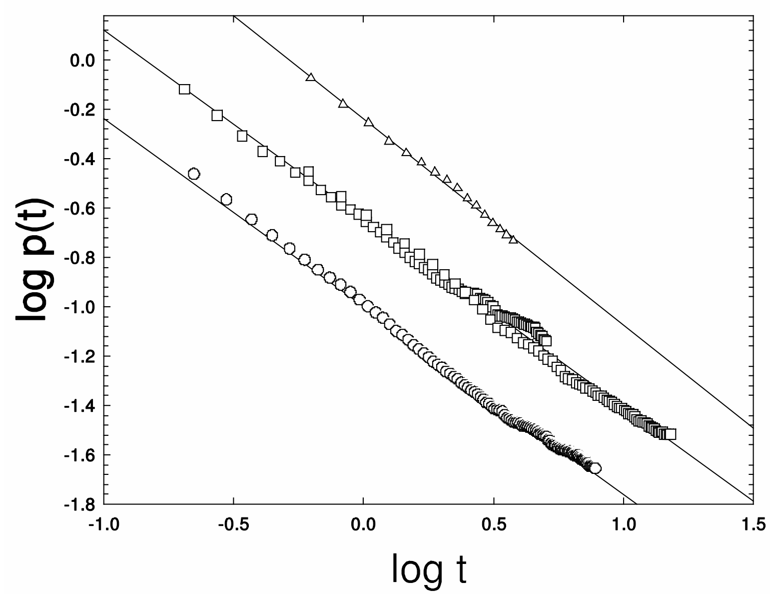
$$P(t_0 \ll t) \sim t^{-\theta_0}, \quad \theta_0(\beta) \qquad \textbf{nontrivial} \qquad \Rightarrow$$



Experiments:

[Dougherty et al., PRL 89, 136102 (2002)]

$\theta_S = 0.77 \pm 0.03 \approx 3/4$
$z = 2.17 \pm 0.09 \approx 2$
for Si(111)-($\sqrt{3} \times \sqrt{3}$)-Al
at $T = 770$ K, 870 K, 970 K



Det regner Solen skinner Det sner
Det stormer Vejret er meget forskelligt
Efter der forskellige steder på jorden
Jorden drejer rundt Og engang forsvinder den
Som sand der forsvinder mellem fingrene
Uden at der er nogen fingre
Den forsvinder bare Og sandet forsvinder
Og billedet af jorden som sand der forsvinder forsvinder

Inger Christensen

It rains The sun shines It snows
It storms The weather is very different
According to the different places on earth
The earth turns And once it disappears
Like sand that disappears between the fingers
Without there being any fingers
It just disappears And the sand disappears
And the picture of the world as sand that disappears disappears

Inger Christensen