Surface pattern and scaling study using lattice gas models

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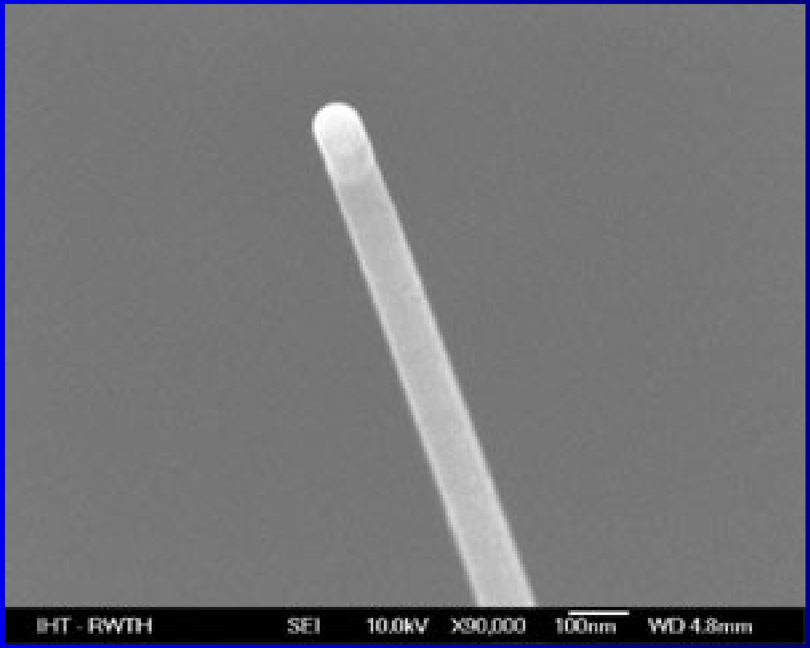
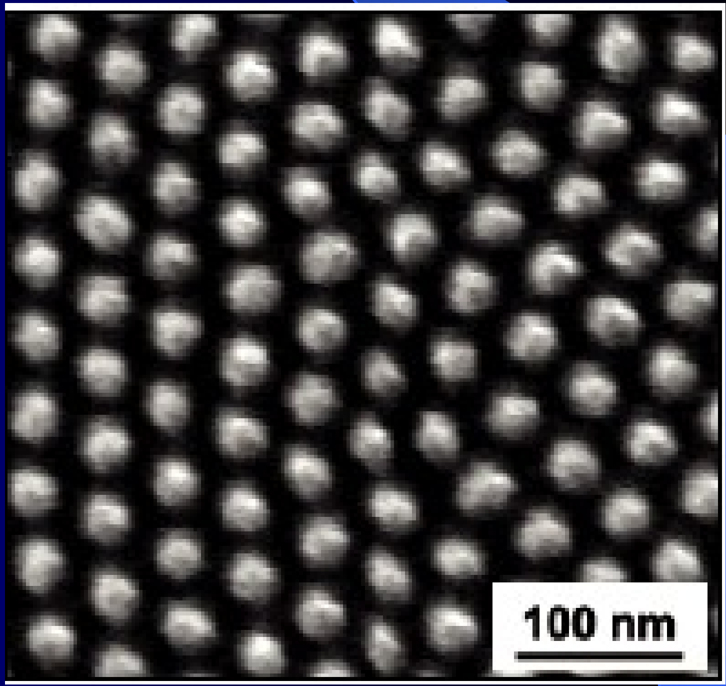
Motivation

In nanotechnologies large areas of **nanopatterns** are needed, which can be fabricated today only by expensive techniques, e.g. electron beam lithography or direct writing with electron and ion beams.



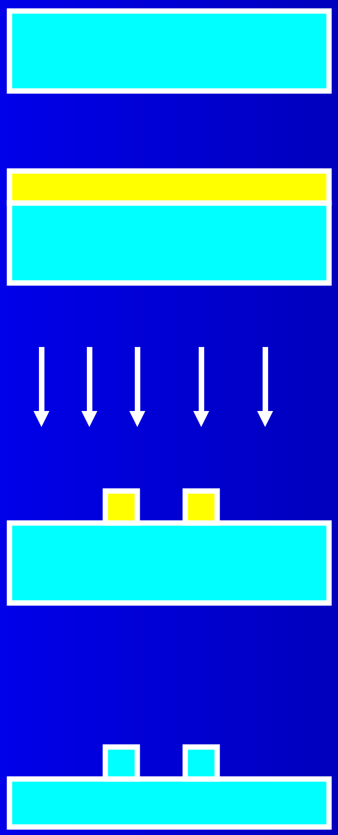
Silicon Nanowire Diameter <100nm



65 billion nanodots per square cm

Top-down Versus Bottom-up approach

Top Down Process



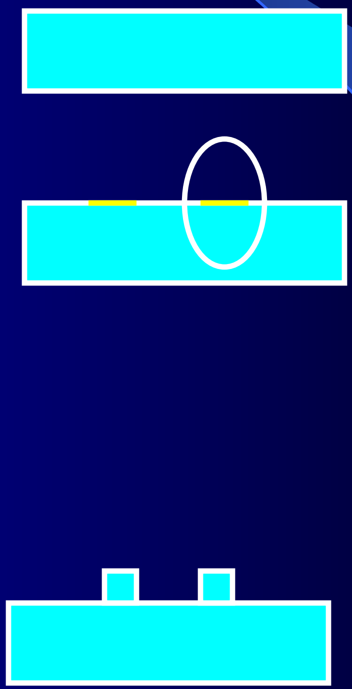
Start with bulk wafer

Apply layer of photoresist

Expose wafer with UV light through mask and etch wafer

Etched wafer with desired pattern

Bottom Up Process



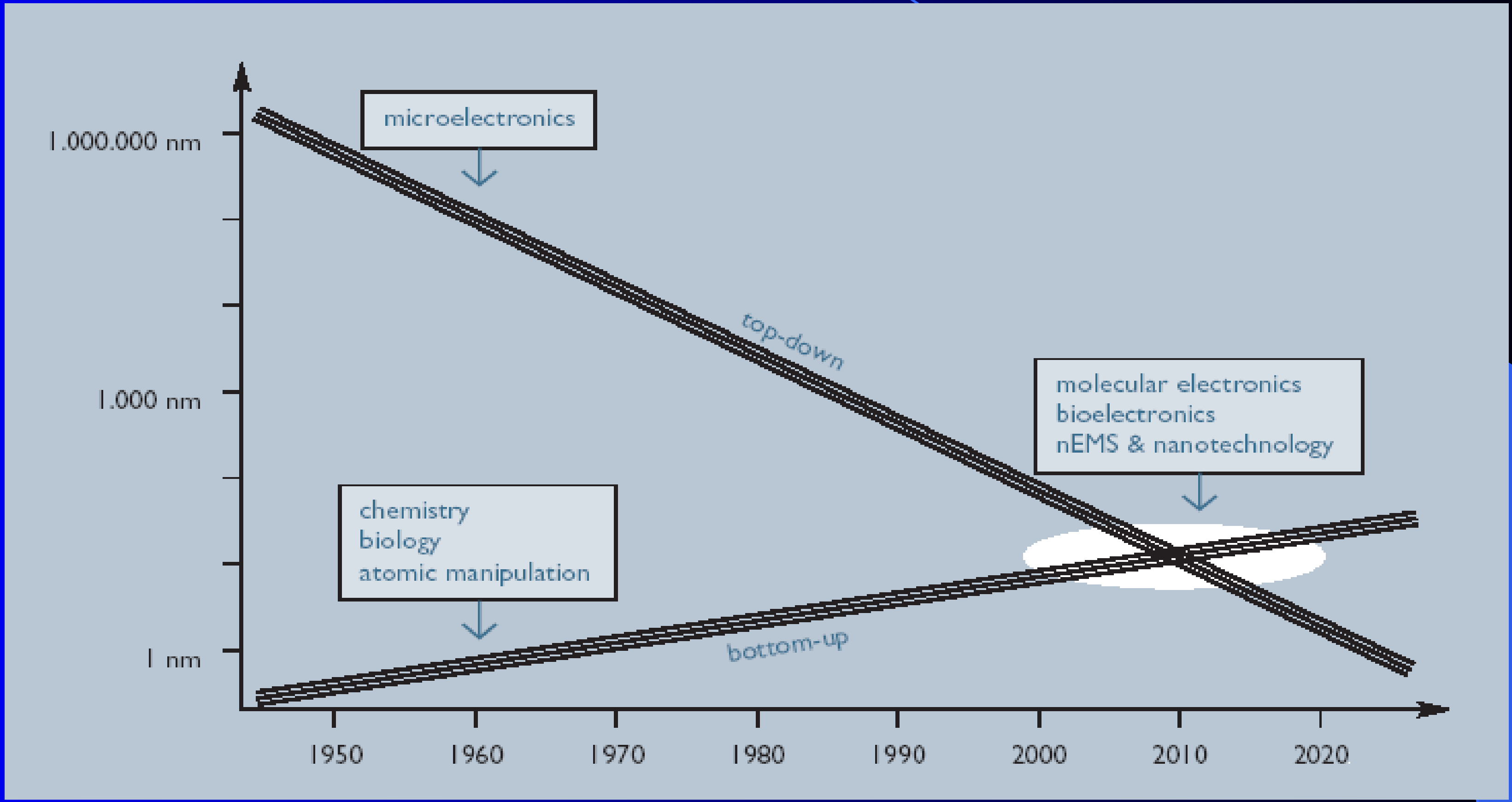
Start with bulk wafer

Alter area of wafer where structure is to be created by adding polymer or seed crystals or other techniques.

Grow or assemble the structure on the area determined by the seed crystals or polymer. (self assembly)

Similar results can be obtained through bottom-up and top-down processes

Future of Top-down and Bottom-Up Processing



http://www.imec.be/wwwinter/business/nanotechnology.pdf

Fundamental theoretical understanding of the ion-beam-induced surface patterning and scaling is needed !

The Kardar-Parisi-Zhang (KPZ) equation/classes

$$\partial_t h(x,t) = v + \sigma \nabla^2 h(x,t) + \lambda(\nabla h(x,t))^2 + \eta(x,t)$$

v, *λ* : mean and local growth velocity
σ : (smoothing) surface tension coefficient
η : roughens the surface by a zero-average Gaussian noise field:

$$<\eta(x,t)\eta(x',t')> = 2D\,\delta^d(x-x')(t-t')$$

Up-down symmetrical case: $\lambda = 0$: Edwards-Wikinson (EW) equation/classes

The KPZ equation is nonlinear, but exhibits a tilting symmetry as the result of the Galilean invariance:

$$h \to h' + \epsilon \mathbf{x}, \qquad \mathbf{x} \to \mathbf{x}' - \lambda \epsilon t, \qquad t \to t' \tag{7.26}$$

where ϵ is an infinitesimal angle. As a consequence the scaling relation

$$\tilde{\alpha} + Z = 2 \tag{7.27}$$

The Kardar-Parisi-Zhang (KPZ) equation/classes

Exactly solvable in *1+1 d* but, in higher dimension even field theory failed due to not being able to access the strong coulping regime:

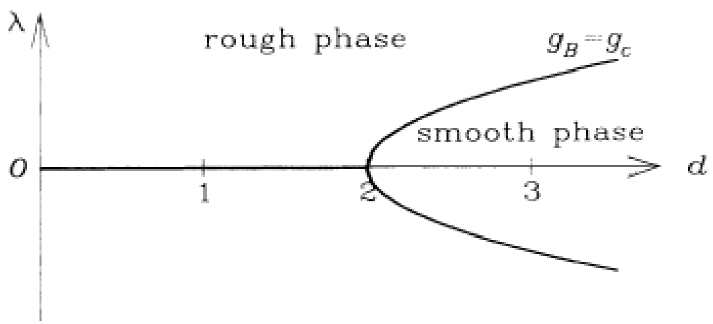


FIG. 1. Schematic phase diagram of the KPZ equation from the one-loop RG analysis. Transitions are marked by thick lines.

Table 7.2 Scaling exponents of KPZ classes.

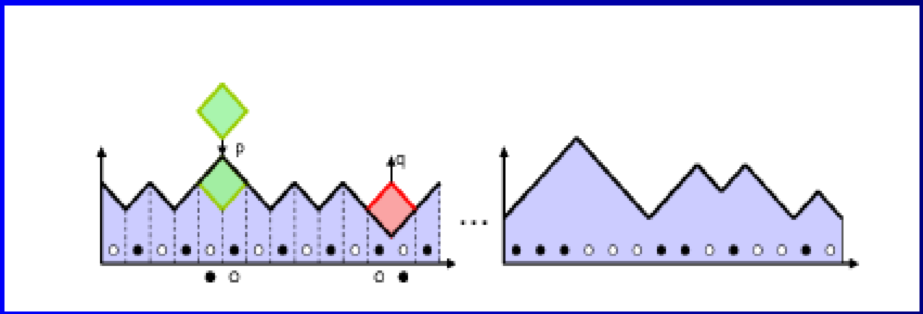
d	$\tilde{\alpha}$	$\tilde{\beta}$	Z
1	1/2	1/3	3/2
2	0.38	0.24	1.58
3	0.30	0.18	1.66

The upper critical dimension is still debated: $d_c = 2, 4, \ldots \infty$?

2-dim numerical estimates have a spread*:* $\alpha = 0.36 - 0.4$

Field theoretical conjecture by *Lässig :* $\alpha = 2/5$

Mappings of KPZ onto lattice gas system in *1d*



Kawasaki exchange of particles

- Mapping of the *1+1* dimensional surface growth onto the 1d ***ASEP*** model.
- Surface attachment (with probability ***p***) and detachment (with probability ***q***) corresponds to anisotropic diffusion of particles (bullets) along the *1d* base space (*M. Plischke, Rácz and Liu, PRB 35, 3485 (1987*))

One of the simplest DDS is the one-species, asymmetric simple exclusion process (**ASEP**) (see Fig. 3.1). This is a site restricted, RD model with

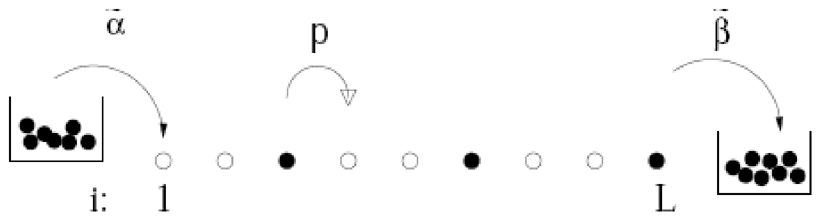


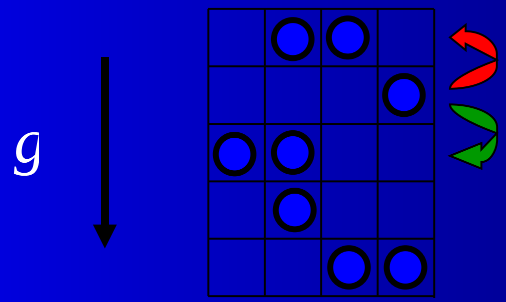
Fig. 3.1 Dynamics of the ASEP with particle injection (rate $\tilde{\alpha}$) at the left and removal (rate $\tilde{\beta}$) at the right boundary.

The simple ***ASEP*** is exactly soved and many features (response to disorder, different boundary conditions ...) are known.

Driven Ising Lattice Gas

invented twenty five years ago (*Katz,Lebowitz,Sphon*)

- Take the well-known equilibrium Ising system
- Drive it far from thermal equilibrium…….. (by some additional external force, so particles suffer *biased* diffusion.)



Go with rate $e^{-mga/kT}$

Just go!

C : { $n(x,y)$ } with $n = 0,1$

$$\mathbf{H}(\mathbf{C}) = -J \sum_{\boldsymbol{x},\boldsymbol{a}} n(\boldsymbol{x})\, n(\boldsymbol{x}+\boldsymbol{a})$$

- Broken detailed balance condition:

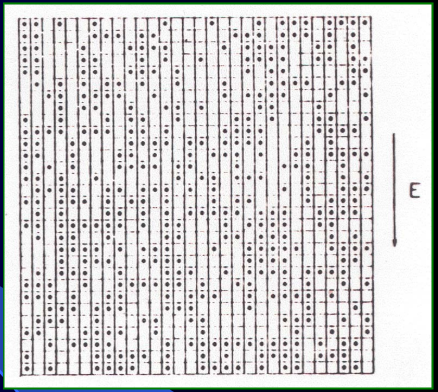
$$R(\mathbf{C} \to \mathbf{C}') \,/\, R(\mathbf{C}' \to \mathbf{C}) \neq exp[\{\mathbf{H}(\mathbf{C}') - \mathbf{H}(\mathbf{C})\}/kT]$$

- **Stationary distribution, $P^*(\mathbf{C})$, exists…**

...but very different from Boltzmann

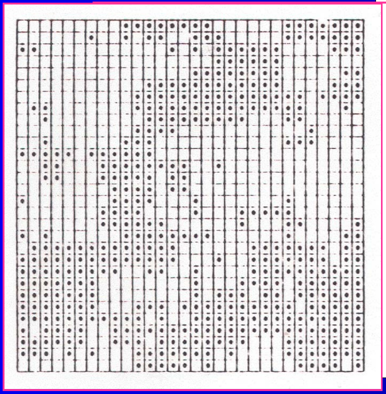
Driven Ising Lattice Gas

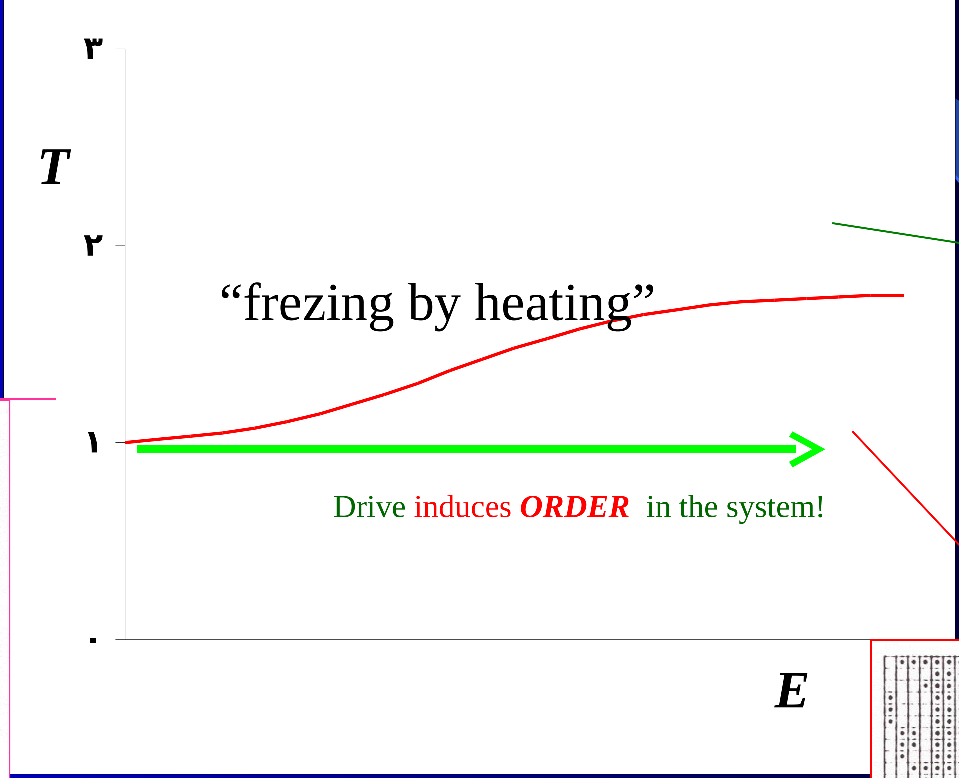
Steady state onfigurations



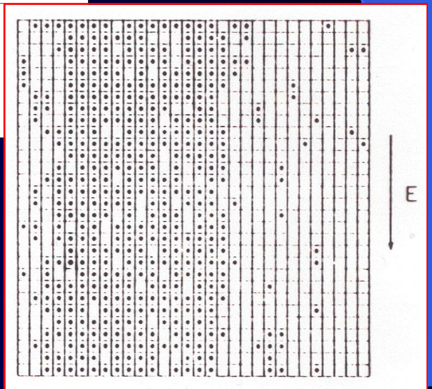
2.2 T_c

1.1 T_c





1.1 T_c



Stripes can be designed, see for example:

György Szabó, Attila Szolnoki, and Géza Ódor: Orientation in a driven lattice gas Phys. Rev. B 46 (1992) 11 432.

Mappings of KPZ growth in *2+1* dimensions

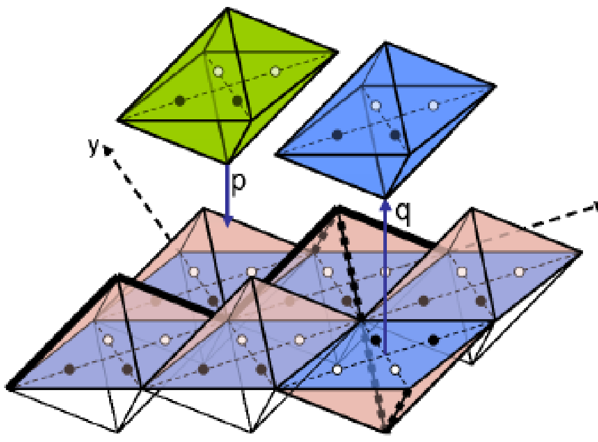


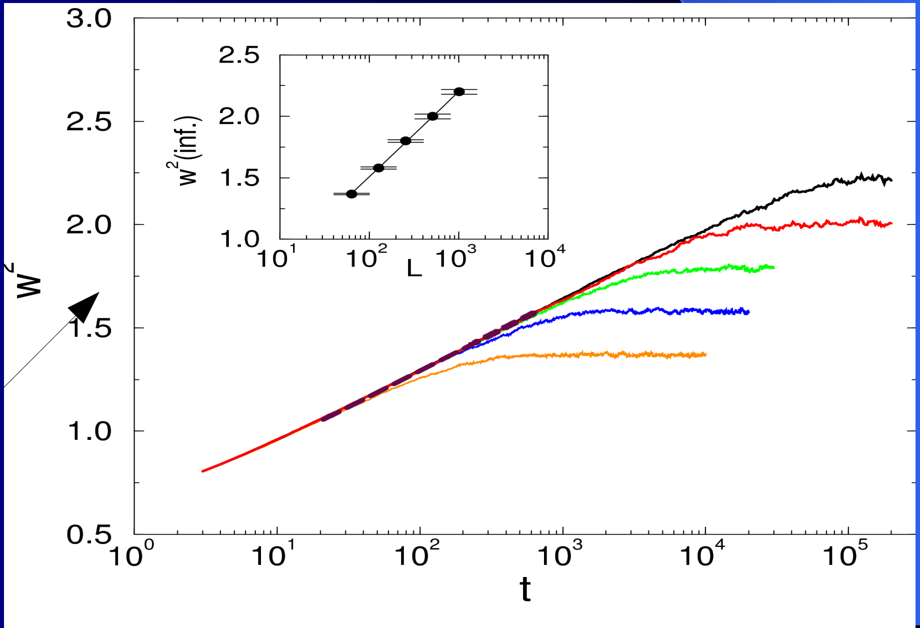
FIG. 2: (Color online) Mapping of the $2+1$ dimensional surface growth onto the $2d$ particle model (bullets). Surface attachment (with probability p) and detachment (with probability q) corresponds to Kawasaki exchanges of particles, or to anisotropic diffusion of dimers in the bisectrix direction of the x and y axes. The crossing points of dashed lines show the base sub-lattice to be updated. Thick solid/dashed lines on the surface show the x/y cross-sections, corresponding to the $1d$ model (Fig. 1.)

- Generalized Kawasaki update:

$$\begin{pmatrix}-1 & 1\\ -1 & 1\end{pmatrix} \rightleftharpoons \begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}$$

- Octahedron model ~ Generalized ASEP: Driven diffusive gas of pairs (dimers)
  (G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009))

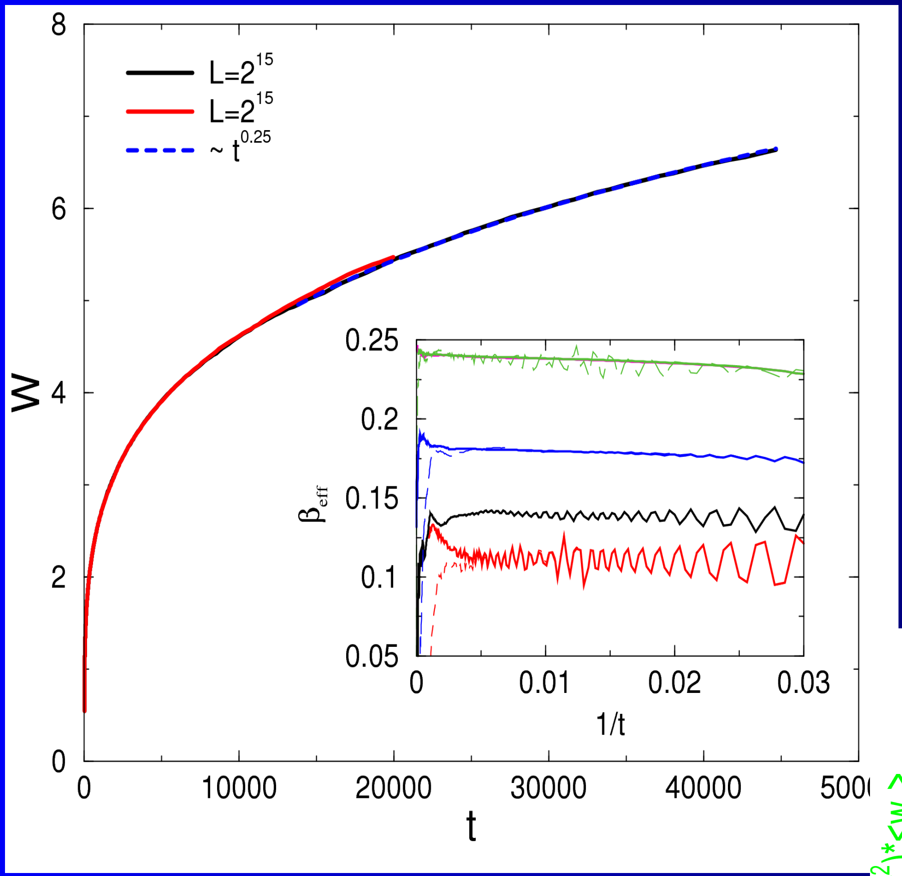
- For *p=q=1* Edwards-Wilkinson (EW) scaling:



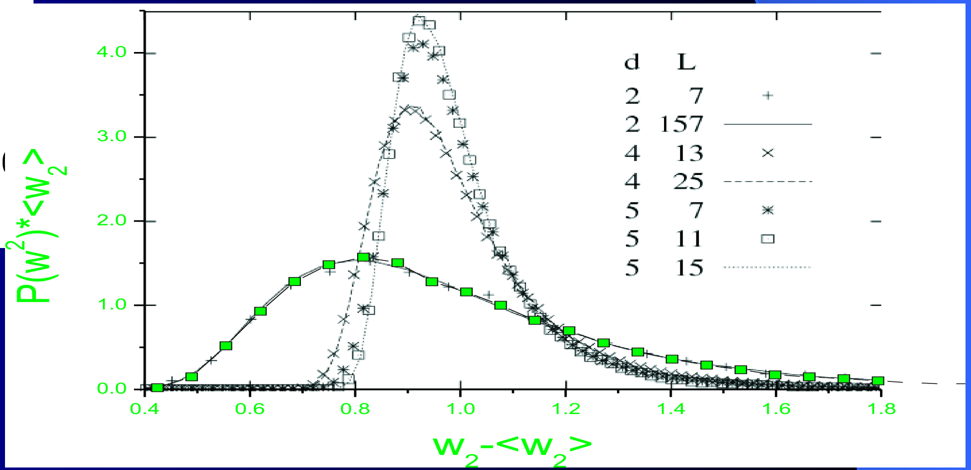
$W^2(t) = 0.152\ \ln(t) + b$ for $t < t_{sat}$

$W^2(L) = 0.304\ \ln(L) + d$ for $t > t_{sat}$

KPZ scaling

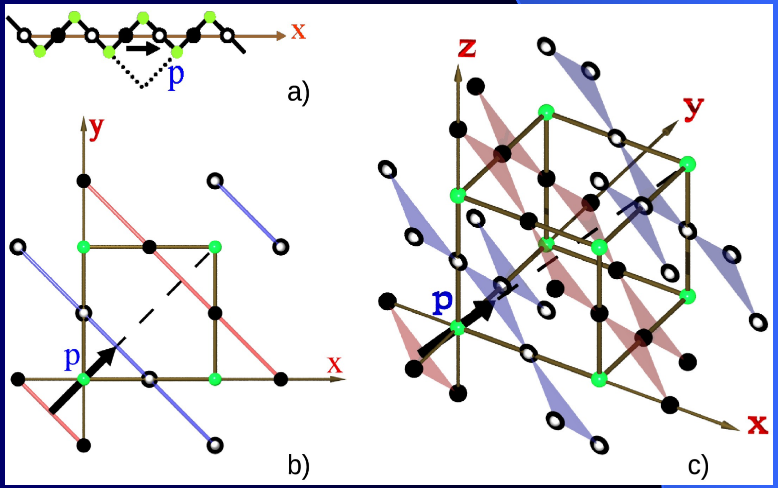


- For *p=1, q=0* KPZ scaling:
  $W(t) \sim t^{0.245(5)}$ for $t < t_{sat}$
  $W(L) \sim L^{0.395(5)}$ for $t > t_{sat}$
- Conciliation with the field theoretical prediction by Lassig: $\beta = 1/4,\ \alpha = 4/10,\ z = 1.6$
- The $P(W^2)$ distribution agrees with that of *Marinari et al.*:



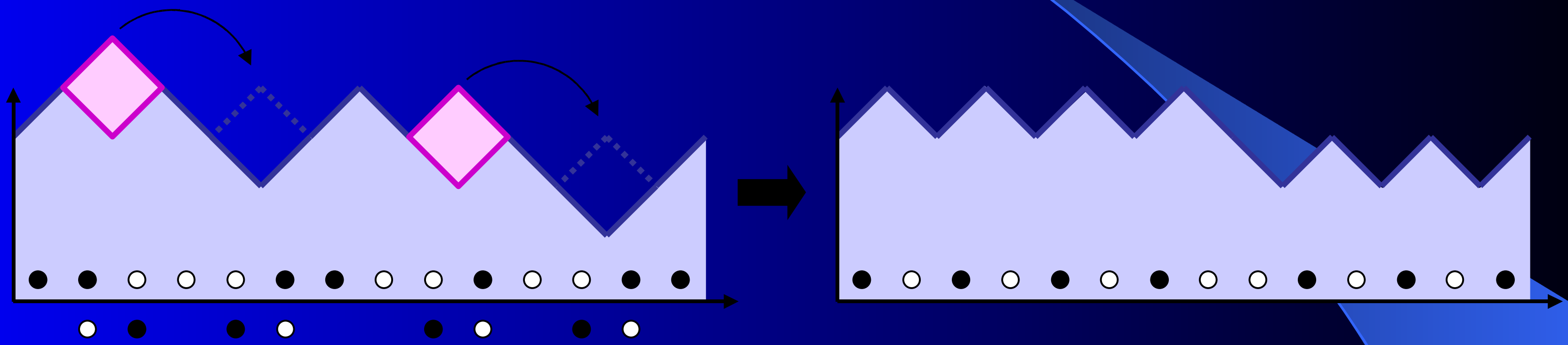
In higher dimensions

- Effective, bit-coded simulations of driven Ising-like lattices ⇒ Precise numerical estimates on large size lattices
- Generalization of the rooftop (octahedron) model in higher dimensions (*3*,*4*,*5*) is done (*64*^{5} sized lattices!)
- In *d* dimensions: *KPZ* ~ spatially anisotropic, driven random walk of oriented *d-mers* ⇒ Topological exclusion effects make them nontrivial
- Upper-critical dimension: Irrelavancy of topological constraints above a **finite** $\boldsymbol{d_c}$?
- *G.Ó, B.L, K.H: arXiv:0907.3297*



Pattern formation with the octrahedron model

Competing KPZ and surface diffusion :



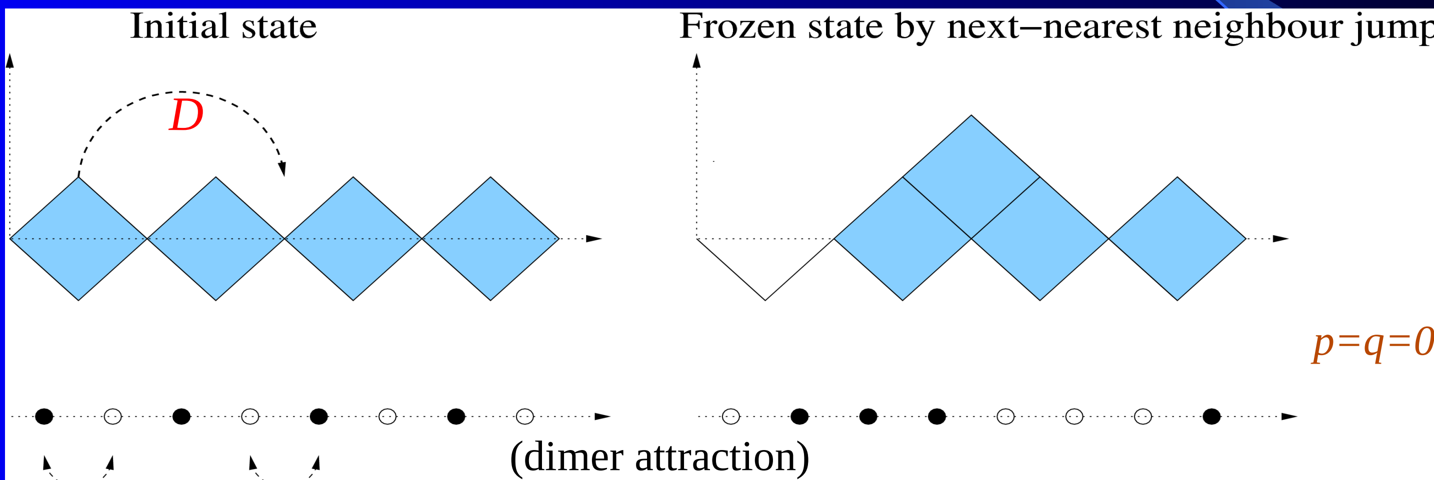
Noisy **Kuramoto-Sivashinsky** equation (KPZ + Mullins Diffusion):

$$\partial_t h(x,t) = \nu + \sigma \nabla^2 h(x,t) + \lambda (\nabla h(x,t))^2 + \kappa \nabla^4 h(h,x) + \eta(x,t)$$

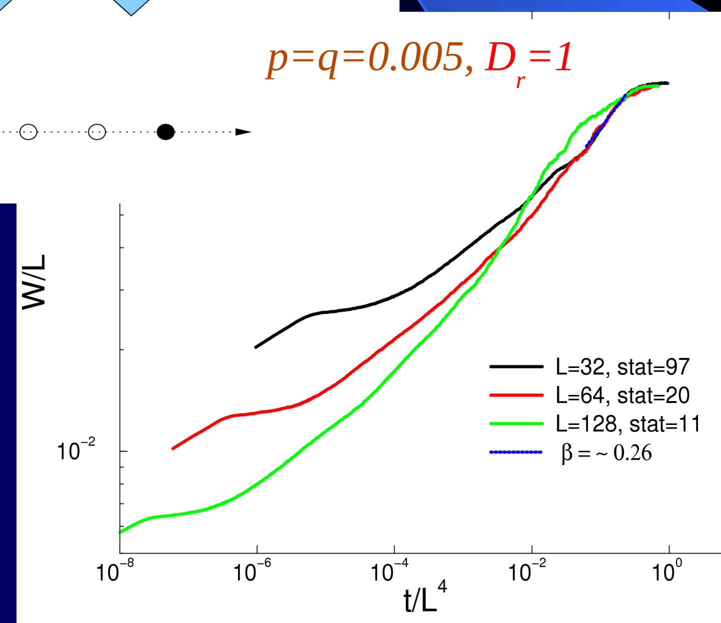
To generate patterns inverse (uphill) diffusion is needed !

Realizing the (inverse) Mullins diffusion

- The pure octahedron MH model realization freezes after intervals of maximal slopes (l_d) is achieved



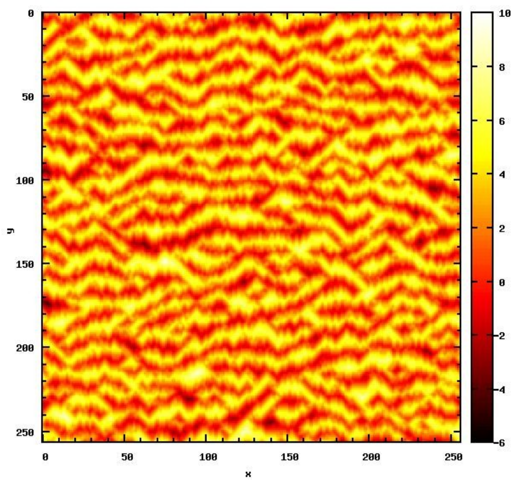
- By an additional small (EW) noise the diffusion can be sustained and Mullins-Herring scaling :
  $\alpha=1$, $\beta=1/4$, $z=4$ is confirmed



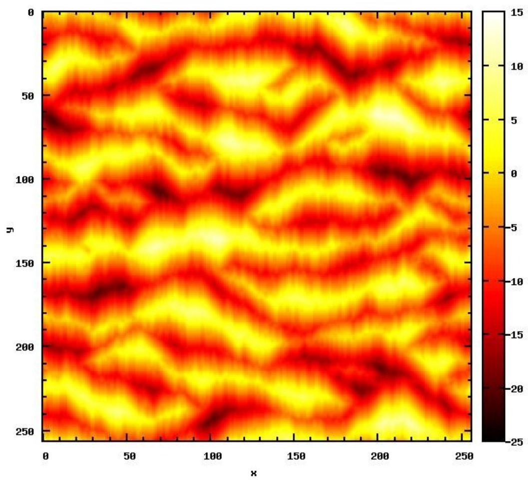
Patterns generated

Anisotropic surface diffusion

10KMCS



30KMCS



Experiment

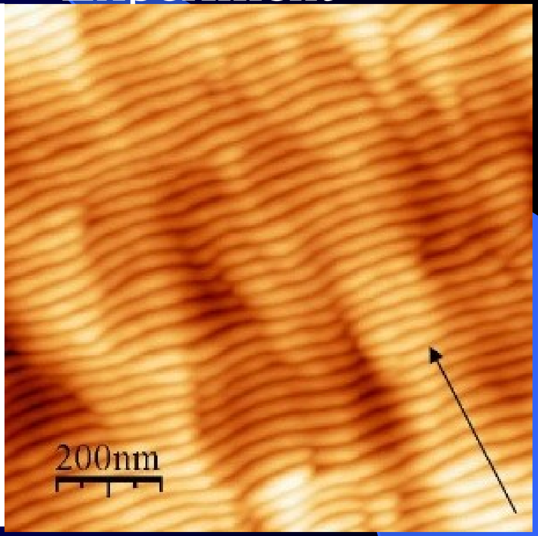


Figure 1 A silicon surface after 500 eV Ar+ sputtering under 67°. The ripples have a periodicity of 35 nm and a height of 2 nm.

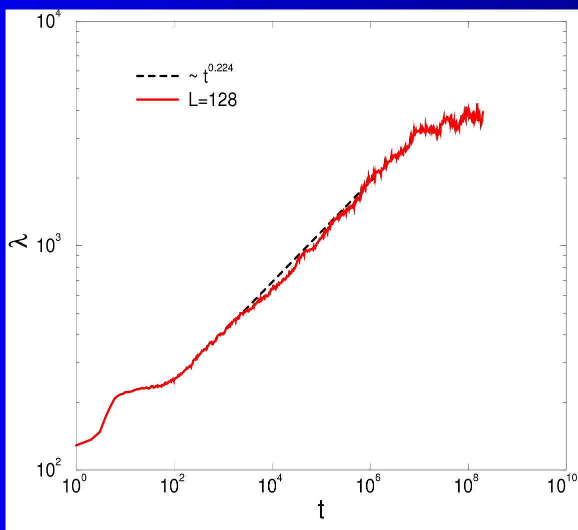
Coarsening ripples

Wavelength growth (scaling) ?

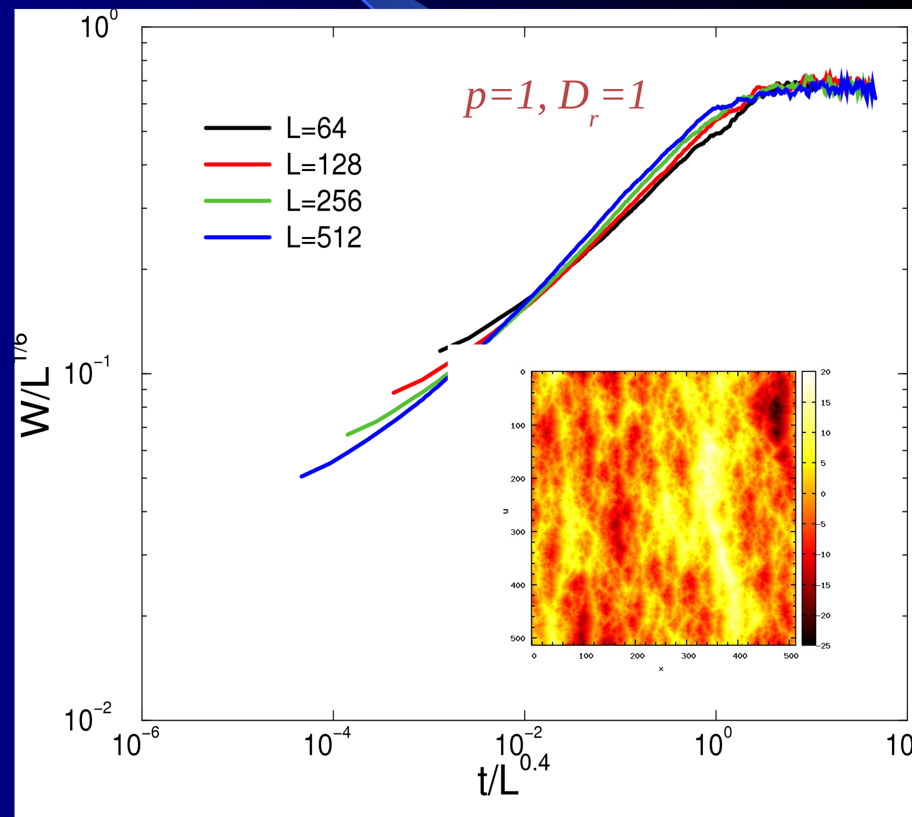
Wavelength growth, inv.MH + KPZ ⇒ KPZ

Anisotropic diffusion

- The wavelenght (defined as longest uniform inteval) grows as:



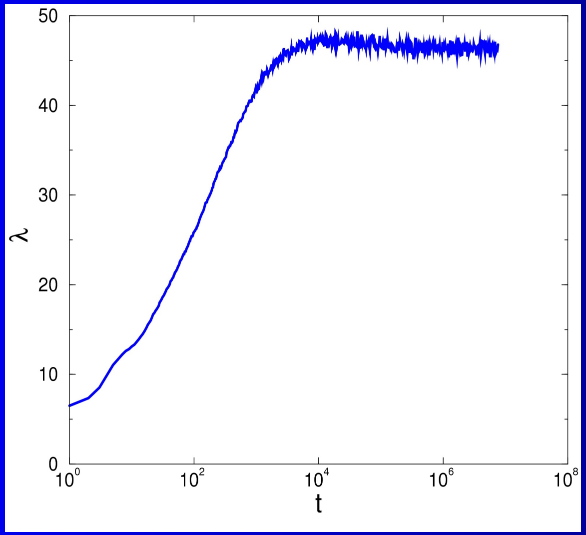
- However if the deposition is strong (*p=1*) we get *AKPZ ~ KPZ* scaling back



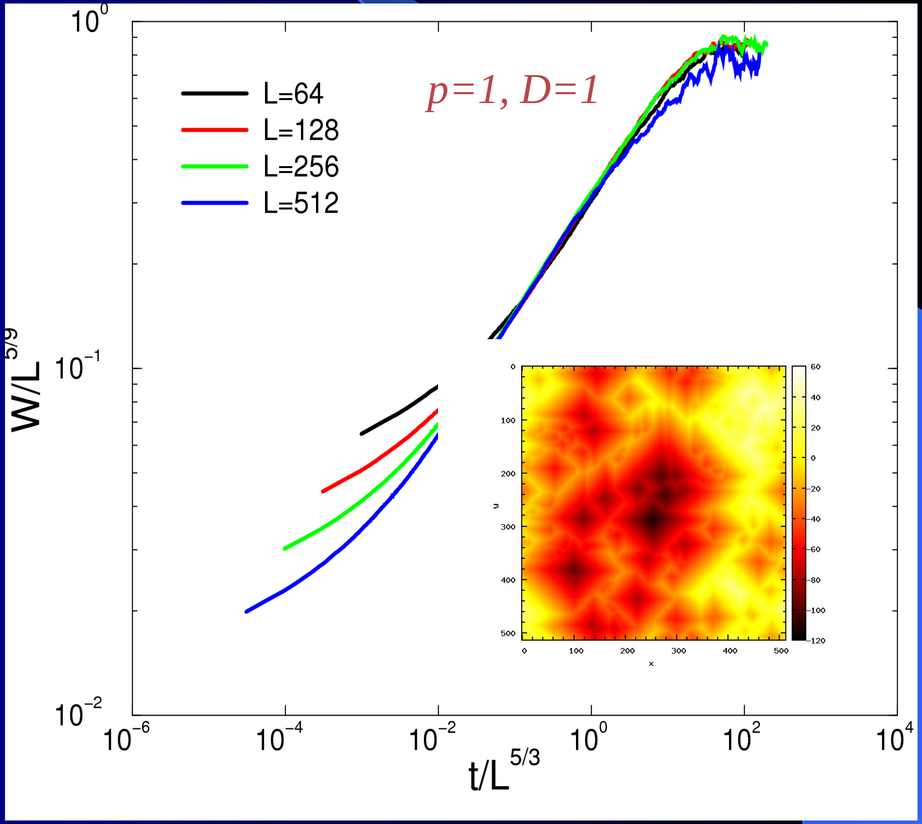
Wavelength, inv.MH + KPZ ⇒ KPZ ?

Isotropic diffusion

- The wavelenght (defined as longest uniform inteval) saturates quickly :



- For strong diffusion (*D=1*) we get (*KPZ ??)* scaling
- For weak diffusion (*D=0.1*) we get *KPZ* scaling

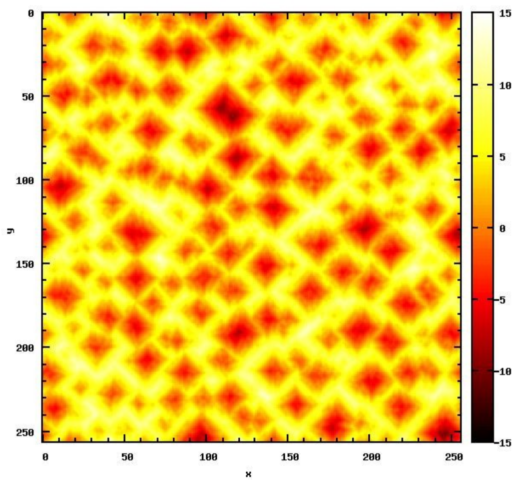


α=5/9, β=1/3, z=5/3 for *L<1024*

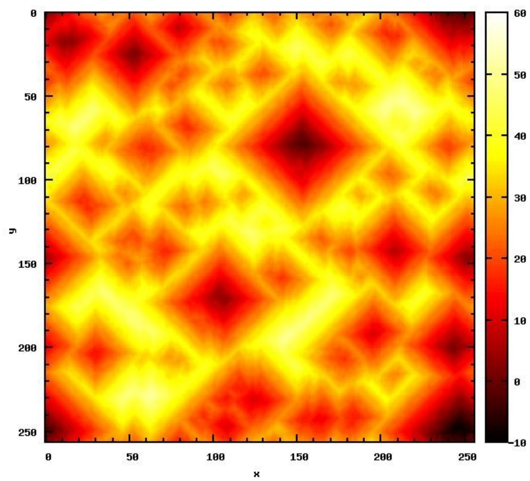
Patterns generated

Isotropic surface diffusion

1KMCS



10KMCS



Experiment

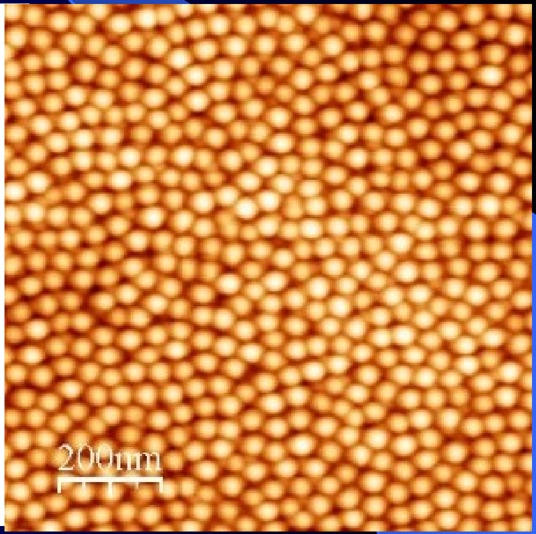
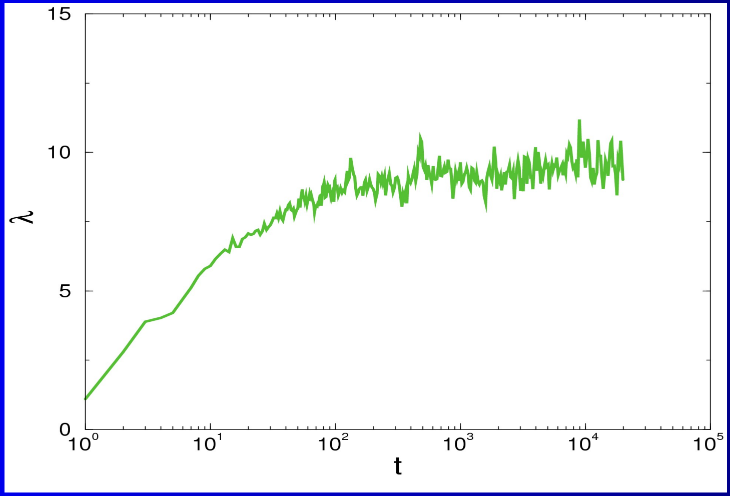


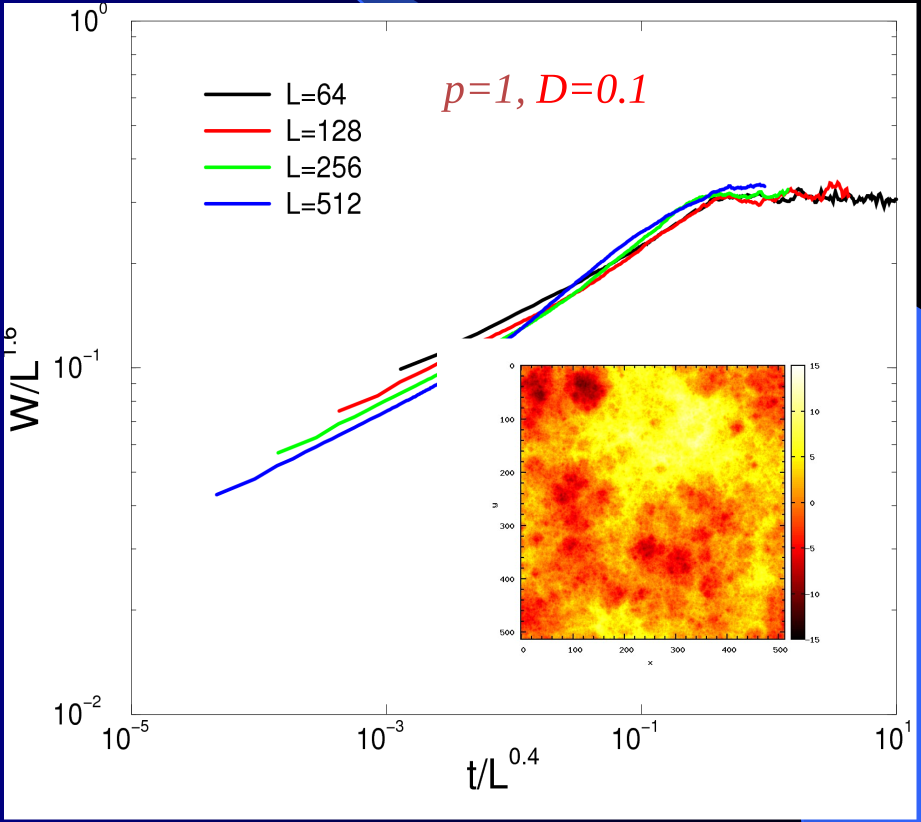
Figure 2 A GaSb surface after normal 500 eV Ar+ sputtering. The periodicity and the height of the dots are both 30 nm.

Coarsening dots

KPZ + Mullins = KS scaling study 1.

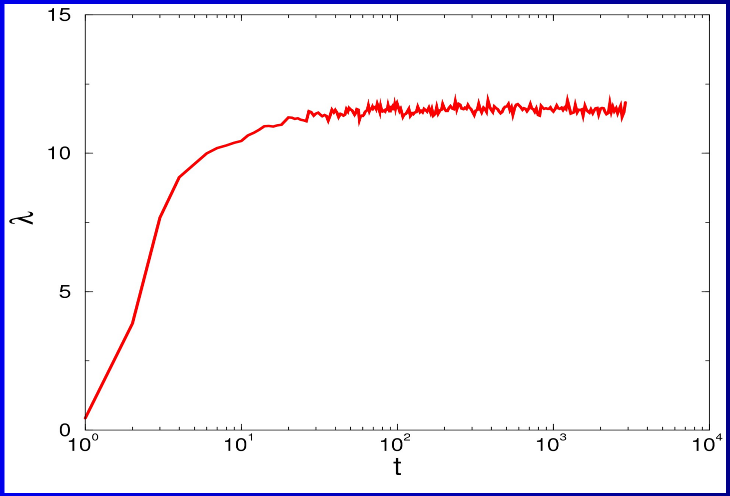
- For **weak** diffusions:
  KS ~ KPZ scaling
  In agreement with field theoretical conjecture for low dimensions
  (Cuerno & Lauritsen '95)
- Wavelenght (defined as longest uniform inteval) saturates quickly to $\lambda_{max} \sim W^2_{max}$

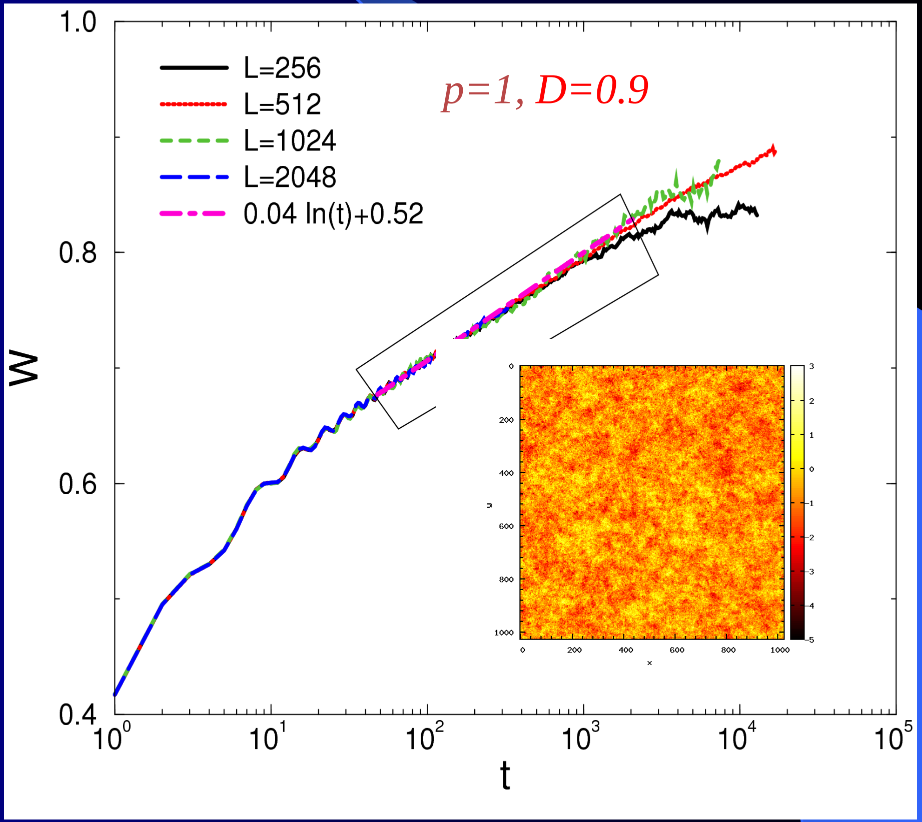




KPZ + Mullins = KS scaling study 2.

- For **strong** diffusions:
  Smooth surface
  Logarithmic growth, but not EW coefficients (a=0.04 ↔ 0.151)
- Wavelenght (defined as longest uniform inteval) saturates quickly to $\lambda \sim 0.001*L$





Summary

Mullins diffusion + KPZ growth

inv.-AD		inv.-D		normal-D	
strong-dep.	weak-dep.	strong-D	weak-D	strong-D	weak-D
KPZ	*MBE*	*KPZ?*	*KPZ*	*EW*	*KPZ*
ripples		dots			

- Precise numerical results for EW, KPZ, KS universality scaling
- Understanding of surface growth phenomena via driven lattice gases
- Efficient method to explore scaling and pattern formation
- Support from grants : DAAD/MÖB D/07/00302, 37-3/2008, OTKA T77629 is acknowledged