RUGOSITE DE SURFACE
Simulations Monte-Carlo
Equations de Langevin

TRAITEMENT
DEPOT
GRAVURE

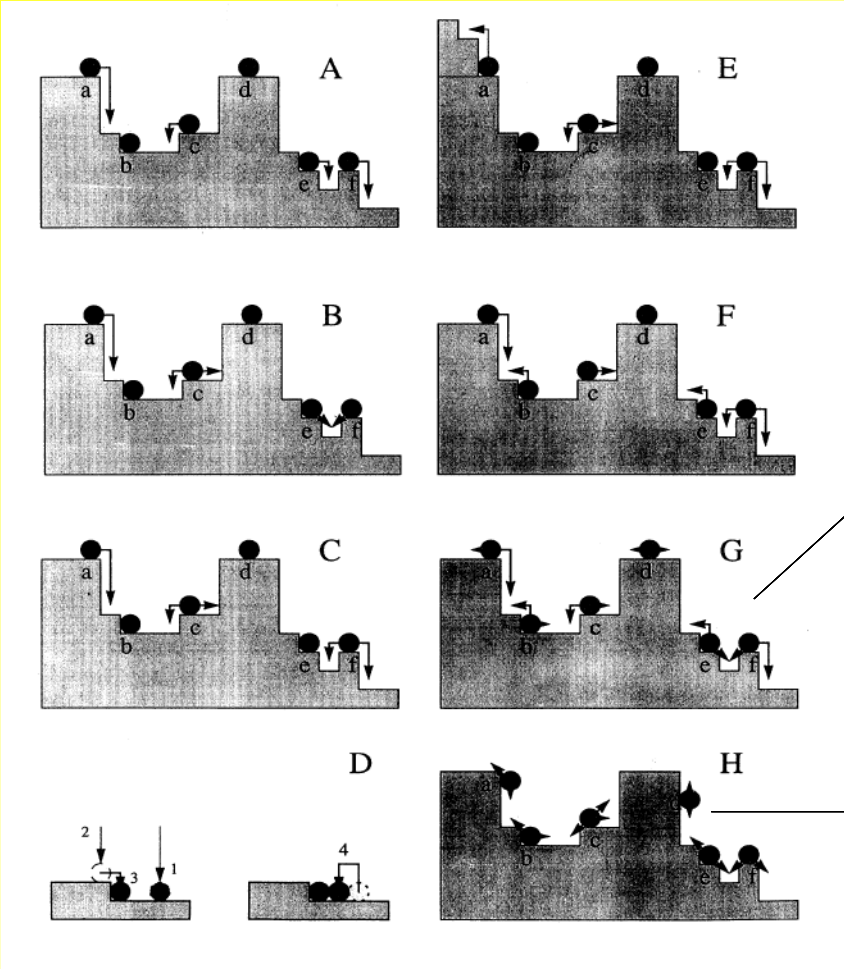
Pascal Brault, Rémi Dussart GREMI
ThuHong VoThi MAPMO Jean-Louis Rouet ISTO

Objectifs

caractériser la rugosité d'une surface:
Dimensions caractéristiques **(⊥ ou //)**

en déduire les mécanismes d'apparition:
Diffusion, redépôt, ...

Simulations Monte-Carlo (SoS)



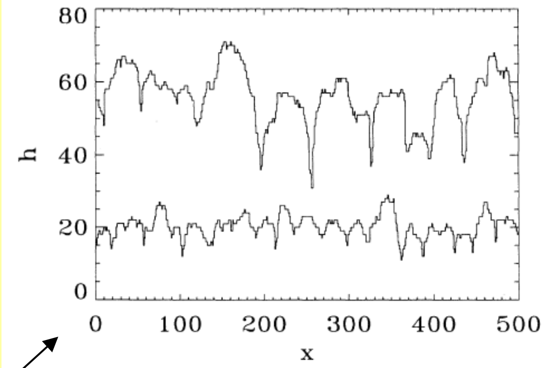


FIG. 12. Morphology of the SOS-MBE surface at $t = 100, 4000$ monolayers at $T = 600$ K, $L = 4000$.

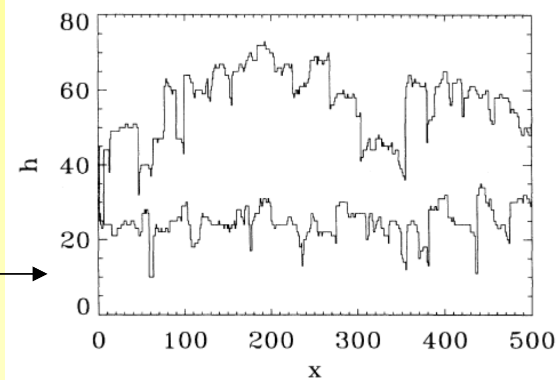
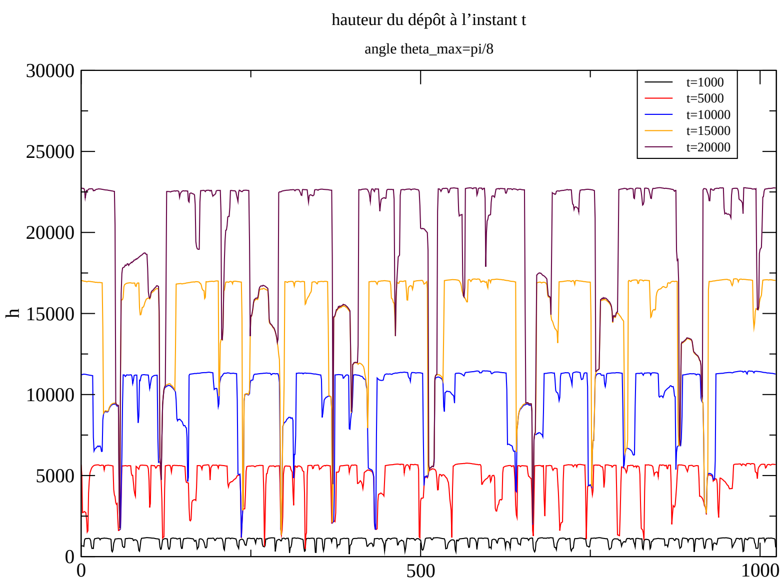


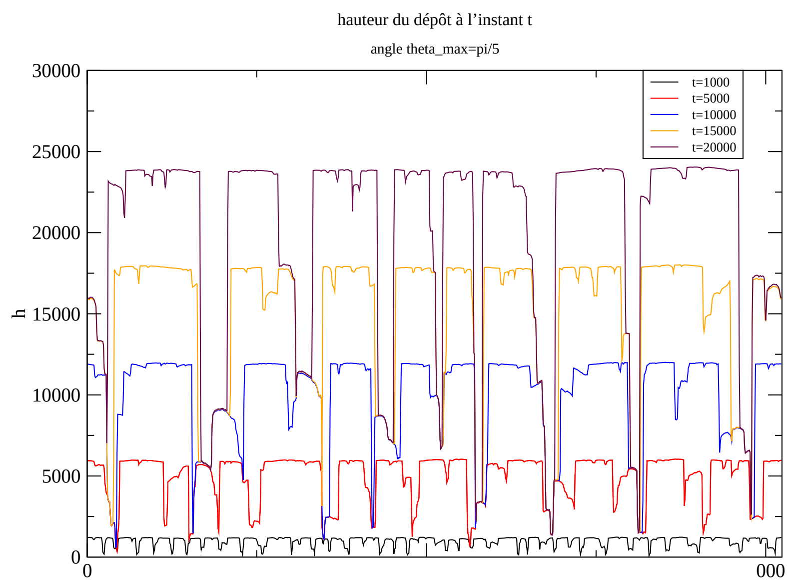
FIG. 13. Morphology of the BD surface at $t = 100, 4000$ monolayers at $T = 600$ K, $L = 4000$.

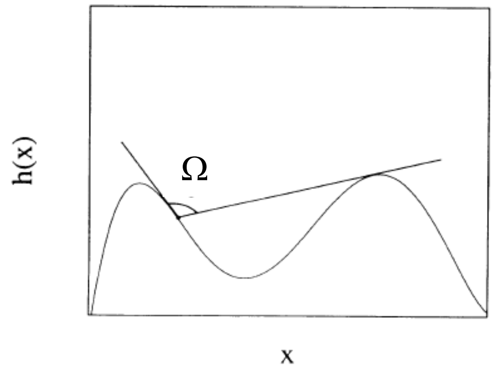
 S.Das sarmas et al, Phys. Rev. E 53, 359 (1996)

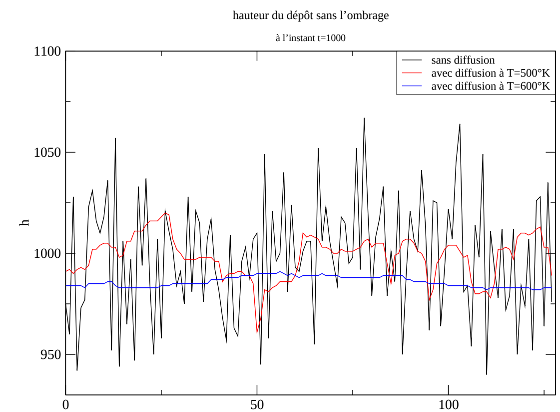
Simulations Monte-Carlo (SoS)

avec ombrage ⇔ atomes proviennent d'un angle solide défini

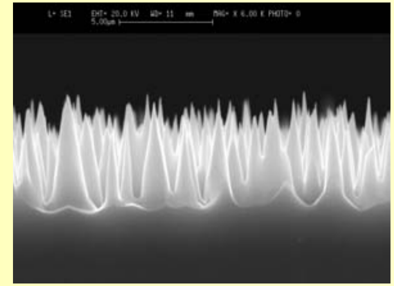








Qu'est ce qui caractérise la rugosité ?



Une surface peut être décrite par une fonction h(x,y,t)

L'amplitude de la rugosité :

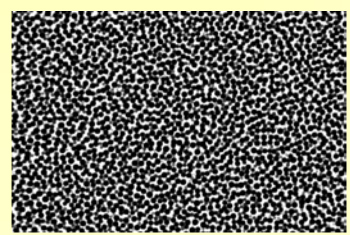
- écart-type → rugosité ⊥

$$\sigma_{\perp}(t) = \left(\frac{1}{NM} \sum_{i=1}^{N-1} \sum_{j=1}^{M-1} \left| h_{ij}(t) - \bar{h}(t) \right|^2 \right)^{\frac{1}{2}} \quad avec \quad \bar{h}(t) = \frac{1}{NM} \sum_{i=1}^{N-1} \sum_{j=1}^{M-1} h_{ij}(t)$$

- Longueur de corrélation → rugosité //

$$\sigma_{//}(t) = \left\langle \left\langle \rho(\vec{r}_0)\, \rho(\vec{r}_0 + \vec{r}) \right\rangle \right\rangle_{|\vec{r}|=r}$$

moyenne sur toutes les origines r_0 et toutes les orientations.
(ρ =1 site occupé, 0 sinon)



Evolution de la rugosité

Il existe des lois d'échelles qui décrivent l'évolution de la rugosité

$$\sigma(L,t) \propto L^{\alpha} f(t/L^{z})$$

$$\sigma \propto L^{\alpha} \qquad \text{for } t \gg L^{z}$$

$$\sigma \propto t^{\beta} \qquad \text{for } t \ll L^{z}, \text{ where } \beta = \frac{\alpha}{z}.$$

$$\zeta \propto t^{1/z} \quad \alpha + z = a + \alpha/\beta = 2$$

$$W(\nu,t) \propto t^{\delta} F(\nu t^{1/z})$$

$$\delta = 2\beta + 2\frac{1}{z} \quad \zeta \propto t^{1/z} \qquad \text{and} \qquad W_0 \propto t^{\delta}$$

Un exemple simple:

croissance de grain sphérique:

$r \propto t^{1/3}$ car dépôt =volume donc $V \propto t$ et $V \propto r^3$

croissance «d'ilôts plats »:

$r \propto t^{1/2}$ car dépôt =surface donc $S \propto t$ et $V \propto r^2$

Equations de Langevin non linéaires (stochastiques)

Equation de conservation

S. Das Sarma et all, Phys Rev E 53, 359 (1996)

Then, apart from the incoming flux, growth must obey a current conservation law defined by

$$\partial h/\partial t = -\boldsymbol{\nabla} \cdot j + \eta(\mathbf{x}, t), \qquad (2.2)$$

where $\mathbf{j}$ is the conserved surface mass current. We emphasize that the generic KPZ nonlinearity is ruled out by the conservation law defined in Eq. (2.2) because $|\boldsymbol{\nabla} h|^2$ cannot be expressed as a divergence. Following Lai and Das Sarma [8] the most general continuum growth equation which preserves current conservation and all the symmetries of the problem (namely, translational invariance along the growth direction and rotational invariance in the substrate plane), can be written as

$$\partial h/\partial t = \nu_2 \nabla^2 h - \lambda_4 \nabla^4 h + \lambda_{22} \nabla^2 (\boldsymbol{\nabla} h)^2$$
$$+ \lambda_{13} \boldsymbol{\nabla} (\boldsymbol{\nabla} h)^3 + \eta(\mathbf{x}, t), \qquad (2.3)$$

$\Rightarrow$ ***Prédire la morphologie de surface***

Equation de conservation (suite)

with the corresponding surface mass current having the form

$$\mathbf{j} = -\nu_2 \nabla h - \lambda_{13}(\nabla h)^3 + \nabla[\nu_4 \nabla^2 h - \lambda_{22}(\nabla h)^2]$$

$$= -(\nabla h)\{\nu_2 + \lambda_{13} |\nabla h|^2\} + \nabla\{\nu_4 \nabla^2 h - \lambda_{22} |\nabla h|^2\}, \tag{2.4}$$

where ν_2, ν_4, λ_{22}, and λ_{13}, the macroscopic growth coefficients, are in principle determined by the growth conditions (e.g., temperature, diffusion length, flux rate) and by the microscopic energetic and kinetic parameters describing the substrate and the growing system. For our purposes $\nu_2, \nu_4, \lambda_{22}, \lambda_{13}$ are simply parameters of the long-wavelength coarse-grained continuum theory. Note that the current $\mathbf{j}$ is written as a sum of two terms in Eq. (2.4), the first of which arises from a generalized surface tension and the second term arises from a generalized (nonequilibrium) chemical potential.

Equations de Langevin non linéaires (stochastiques)

Signification géométrique

Z. W. Lai and S. Das Sarma, Phys Rev Lett 66, 2348 (1991)

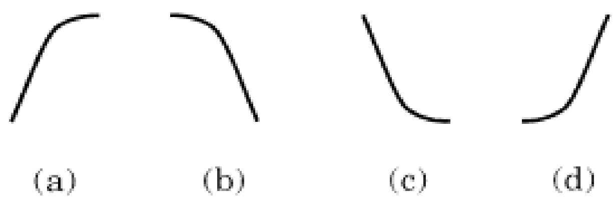


FIG. 1. Any small segment of the coarse-grained surface must have increasing, decreasing, or constant slopes and thus falls into one of the four topologically different basic building blocks as shown. The straight-line segments are just the topological extension of the two ends of the building blocks.

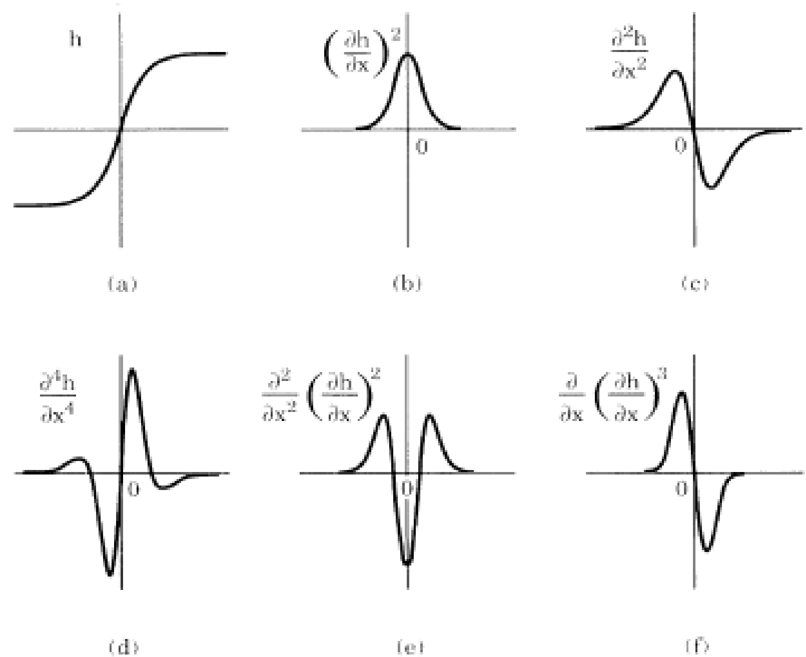


FIG. 2. (a) A typical segment of surface by combining building blocks (a) and (d) of Fig. 1. (b)–(f) Various derivatives of (a) as labeled.

$$\partial h/\partial t = \nu_2 \nabla^2 h + \lambda_2 |\nabla h|^2 + \eta(\mathbf{x}, t), \qquad (2.1)$$ KPZ

$$\partial h/\partial t = \nu_2 \nabla^2 h + \eta(\mathbf{x}, t). \qquad (2.5)$$ EW

$$\partial h/\partial t = -\lambda_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta(\mathbf{x}, t). \qquad (2.10)$$ MBE

$$\partial h/\partial t = -\lambda_4 \nabla^4 h + \eta(\mathbf{x}, t), \qquad (2.11)$$ (*)

$$\partial h/\partial t = -\lambda_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \lambda_{13} \nabla (\nabla h)^3 + \eta(\mathbf{x}, t). \qquad (2.12)$$ (**)

Dimension	1 + 1			2 + 1		
Exponent	α	z	β	α	z	β
$\nabla^2 h$—Eq. (2.5)	1/2	2	1/4	0 (log)	2	0 (log)
$(\nabla h)^2$—Eq. (2.1)	1/2	3/2	1/3	~ 0.4	~ 1.67	~ 0.24
$\nabla^4 h$—Eq. (2.11)	3/2	4	3/8	1	4	1/4
$\nabla^2(\nabla h)^2$—Eq. (2.10)	1	3	1/3	2/3	10/3	1/5
$\nabla(\nabla h)^3$—Eq. (2.12)	3/4	5/2	3/10	1/2	3	1/6

(*) nonconserved surface diffusion

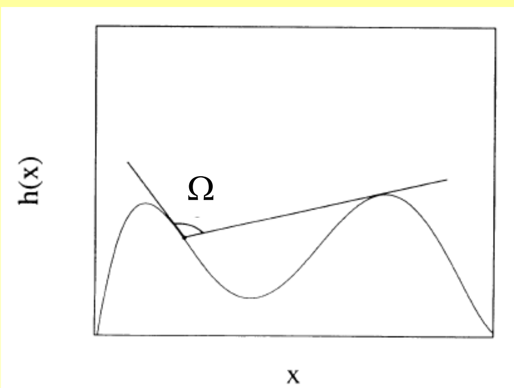
(**) conserved surface diffusion

Equations de Langevin non linéaires (stochastiques)

$$\frac{\partial h(r,t)}{\partial t} = D_s \nabla^4 h(r,t) + D_v \nabla^3 h(r,t) + \nu \nabla^2 h(r,t) + \lambda(\nabla h(r,t))^2 + R\Omega(h,t) + \eta(r,t)$$

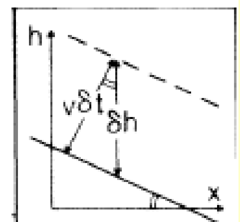
R= taux de gravure, Ω angle d'ouverture (ombrage), D_s = diffusion de surface,
D_v = diffusion dans le volume, λ = croissance oblique,
ν = évaporation-redépôt, η = bruit aléatoire

Ombrage



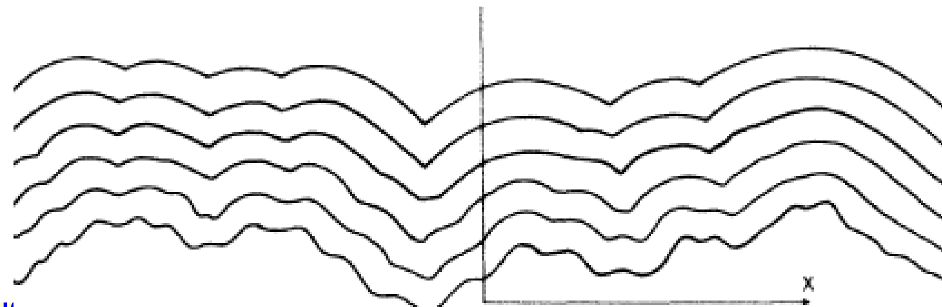
non-linéarité
Eq^n KPZ

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta(\mathbf{x},t).$$



$$\delta h = \sqrt{(R\delta t)^2 + (R\delta t \nabla h)^2}\,;\ \alpha = \nabla h;$$

$$\Rightarrow \frac{\partial h}{\partial t} = R\sqrt{1+(\nabla h)^2} \approx R + \frac{R}{2}(\nabla h)^2 + \cdots$$



Equations de Langevin non linéaires (stochastiques)

A propos de Kardar Parisi Zhang Phys.Rev Lett.56, 889 (1986)

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta(\mathbf{x},t). \qquad \langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2D\delta^d(\mathbf{x}-\mathbf{x}')\delta(t-t'),$$

$$W(\mathbf{x},t) = \exp[(\lambda/2\nu)h(\mathbf{x},t)], \Rightarrow \partial W/\partial t = \nu\nabla^2 W + (\lambda/2\nu)\eta(\mathbf{x},t)W,$$

$$\mathbf{v} = -\nabla h, \Rightarrow \partial \mathbf{v}/\partial t + \lambda \mathbf{v}\cdot\nabla\mathbf{v} = \nu\nabla^2\mathbf{v} - \nabla\eta(\mathbf{x},t),$$

($\lambda = 1 \Rightarrow$ Eq^n de Burger)

Dans (1) si $\eta(\mathbf{x},t) = 0,$ alors $h(\mathbf{x},t) = (2\nu/\lambda)[\ln|\cos(\mathbf{k}\cdot\mathbf{x})| - \nu k^2 t].$

De plus si le profil initial $h(\mathbf{x},0) = h_0(\mathbf{x})$ alors:

$$h(\mathbf{x},t) = \frac{2\nu}{\lambda}\ln\left\{\int_{-\infty}^{\infty}\frac{d^d\xi}{(4\pi\nu t)^{d/2}}\exp\left[-\frac{(\mathbf{x}-\xi)^2}{4\nu t} + \frac{\lambda}{2\nu}h_0(\xi)\right]\right\}.$$

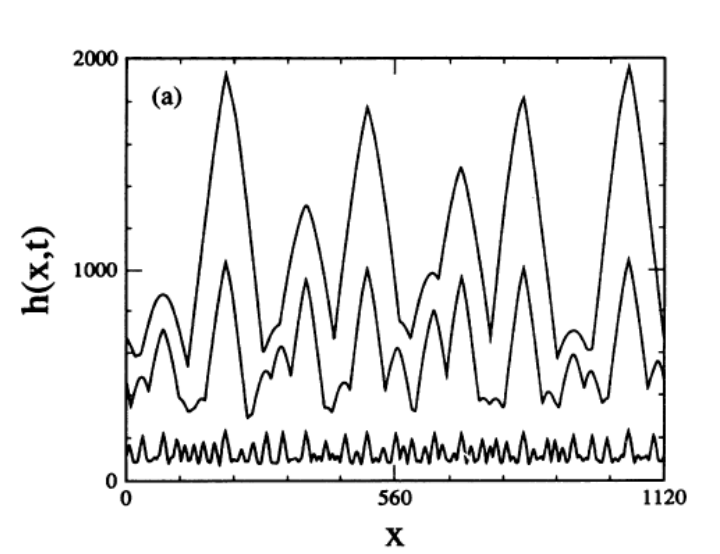
Renormalisation dynamique: E. Medina et al, Phys rev A39,3053 (1989)

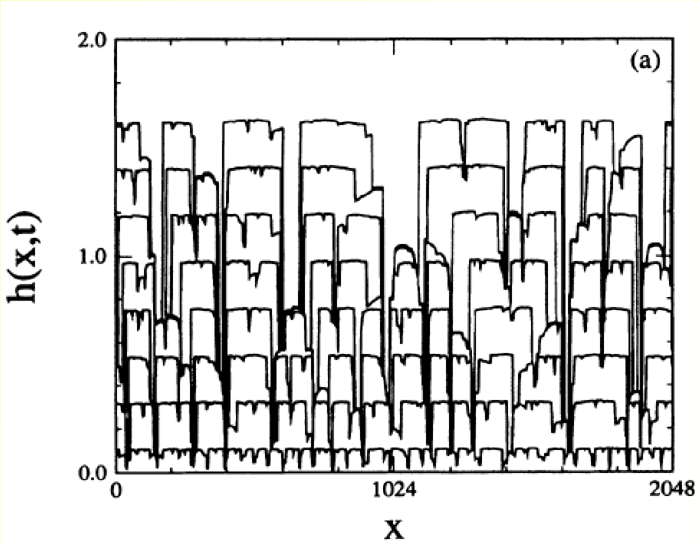
Couplage fort Yan H, Kessler D and Sander L M 1990 *Phys. Rev. Lett.* 64 926

Pb numériques: Lam & shin Phys Rev E57,6506 (1998)

Equations de Langevin non linéaires (stochastiques)

Ombrage





Langevin

Monte-Carlo

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + R\theta(\mathbf{x}, \{h\}) + \eta,$$

Equations de Langevin non linéaires (stochastiques)

Further confirmation of the dramatic effect of evaporation comes from the continuum theory, where the surface is modeled by a smooth, space and time-dependent height function $H(\mathbf{x},t)$. Our starting point is the standard continuum equation for unstable epitaxy [1–3,5–7], to which the leading order effect of desorption is added in terms of a slope-dependent growth rate $V(|\nabla H|)$:

$$\frac{\partial H}{\partial t} = -K\Delta^2 H - \nabla \cdot [f(|\nabla H|^2)\nabla H] + V(|\nabla H|). \qquad (1)$$

Quelques « curiosités »

$$\frac{\partial h}{\partial t} = -\Delta^2 h - \nabla \cdot \{[1-(\nabla h)^2]\nabla h\} - \frac{\alpha^2/3}{1+(\nabla h)^2}.$$

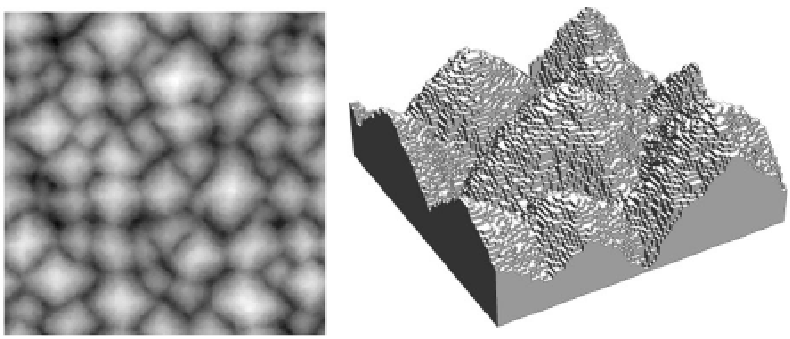
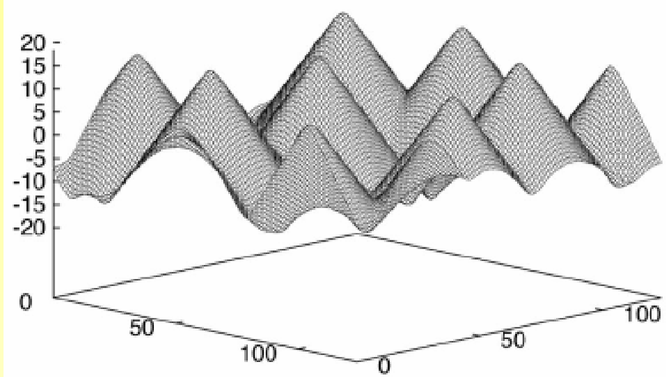


FIG. 2. Surface morphology in KMC simulations after approximately 2000 ML have been deposited. The displayed part of the lattice is 300×300 (plane view, left) and 100×100 (perspective plot, right).



P. Smilauer, PRE59, R6263 (1999)

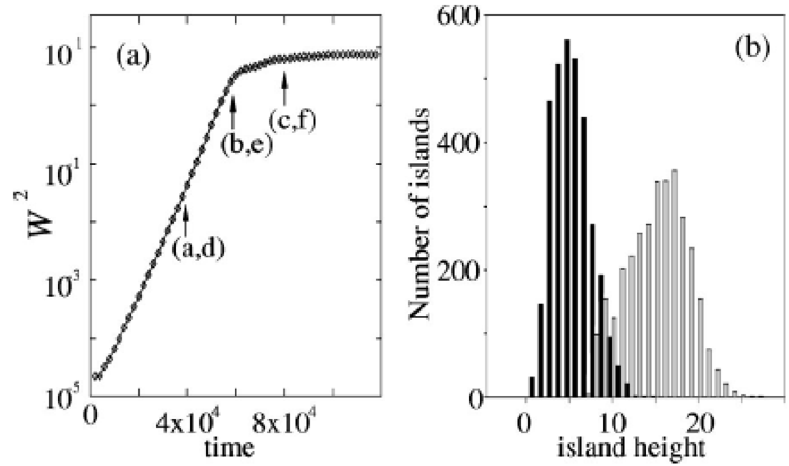
Equations de Langevin non linéaires (stochastiques)

⇒ *Quelques « curiosités »*

$$\partial_t h = \nu_x \partial_x^2 h + \nu_y \partial_y^2 h - D_x \partial_x^4 h - D_y \partial_y^4 h - D_{xy} \partial_x^2 \partial_y^2 h$$

$$+ \frac{\lambda_x}{2} (\partial_x h)^2 + \frac{\lambda_y}{2} (\partial_y h)^2 + \eta(x, y, t),$$

Eq^n de Kuramoto-Sivashinsky)



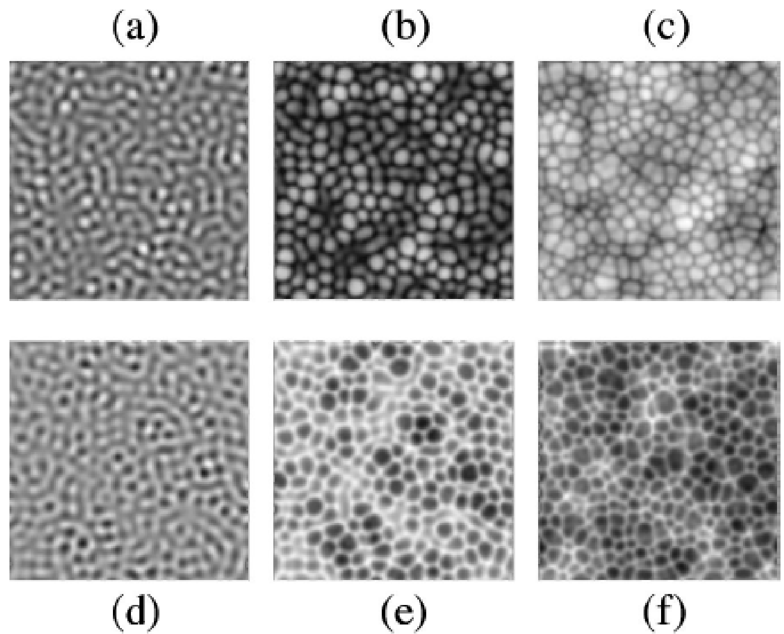
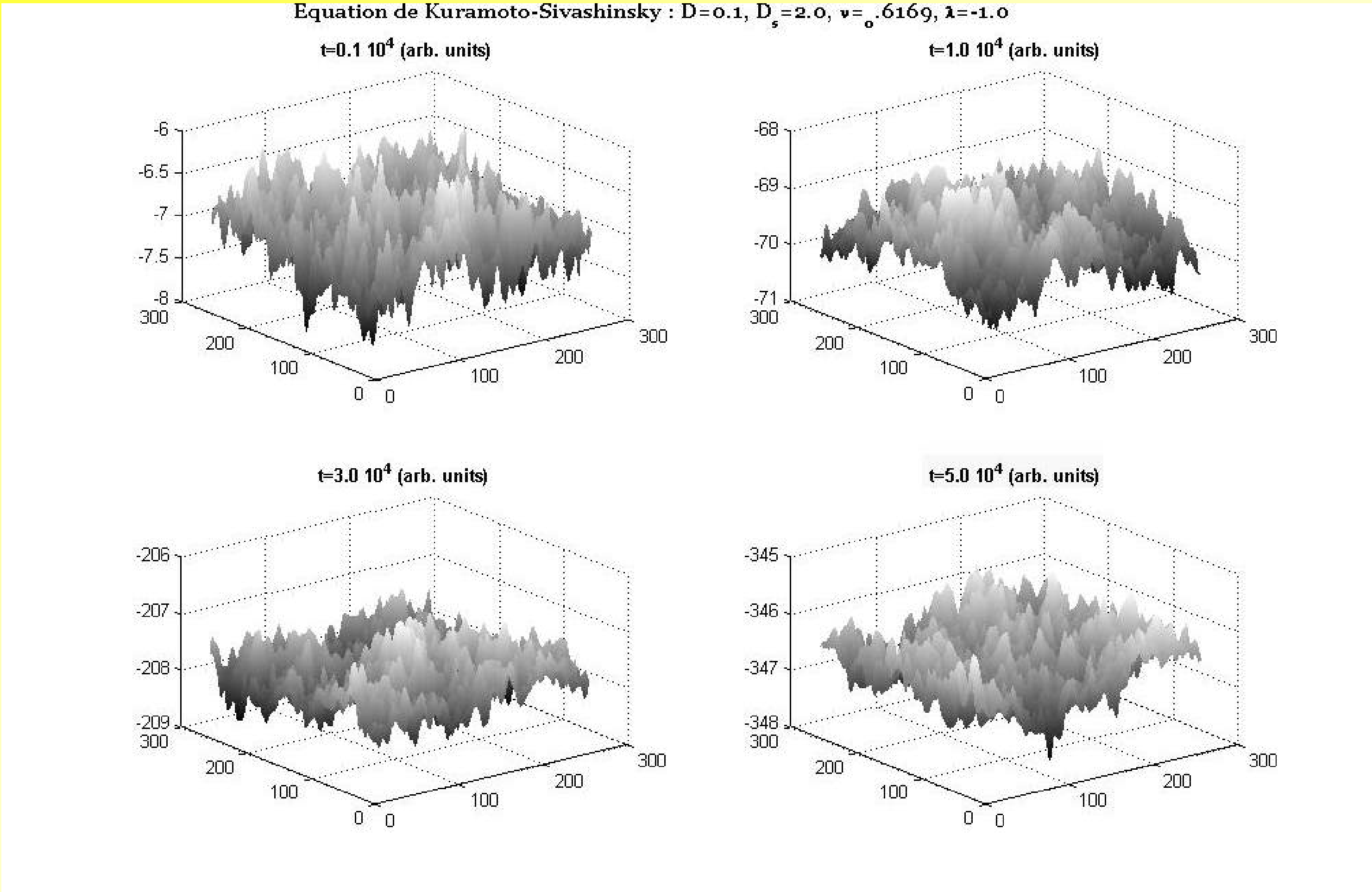


FIG. 2. (a)–(c) Surface morphologies predicted by Eq. (3), for $\lambda = 1$ at different stages of surface evolution. The pictures correspond to (a) $t = 4.0$, (b) 5.8, (c) 8.0×10^4. (d)–(f) The same as in (a)–(c), but for $\lambda = -1$. In all cases we used $\nu = 0.6169$, $D = 2$, and system size 256×256.

B. Khang, APL78, 805 (2001)

KS pour la gravure Cryogénique



Conclusions

- Méthodes MC et équations continue → outils efficaces pour la rugosité
- Recherche de lois universelles → phénomènes analogues
  rugosité ↔ digitation visqueuse
- Elargir les domaines applications au-delà de la MBE.

Pour convaincre de l'utilité des simulations/modélisation auprès des industriels

WHITE PAPER

Modeling and Simulation: The Return on Investment in Materials Science

Sponsored by: Accelrys Inc.

Michael Swenson
Michael Languell, Ph.D.
James Golden, Ph.D.
July 2004