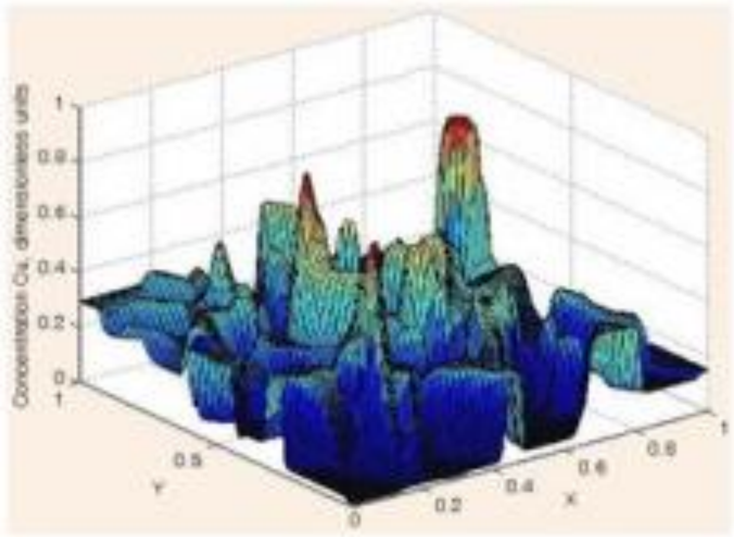


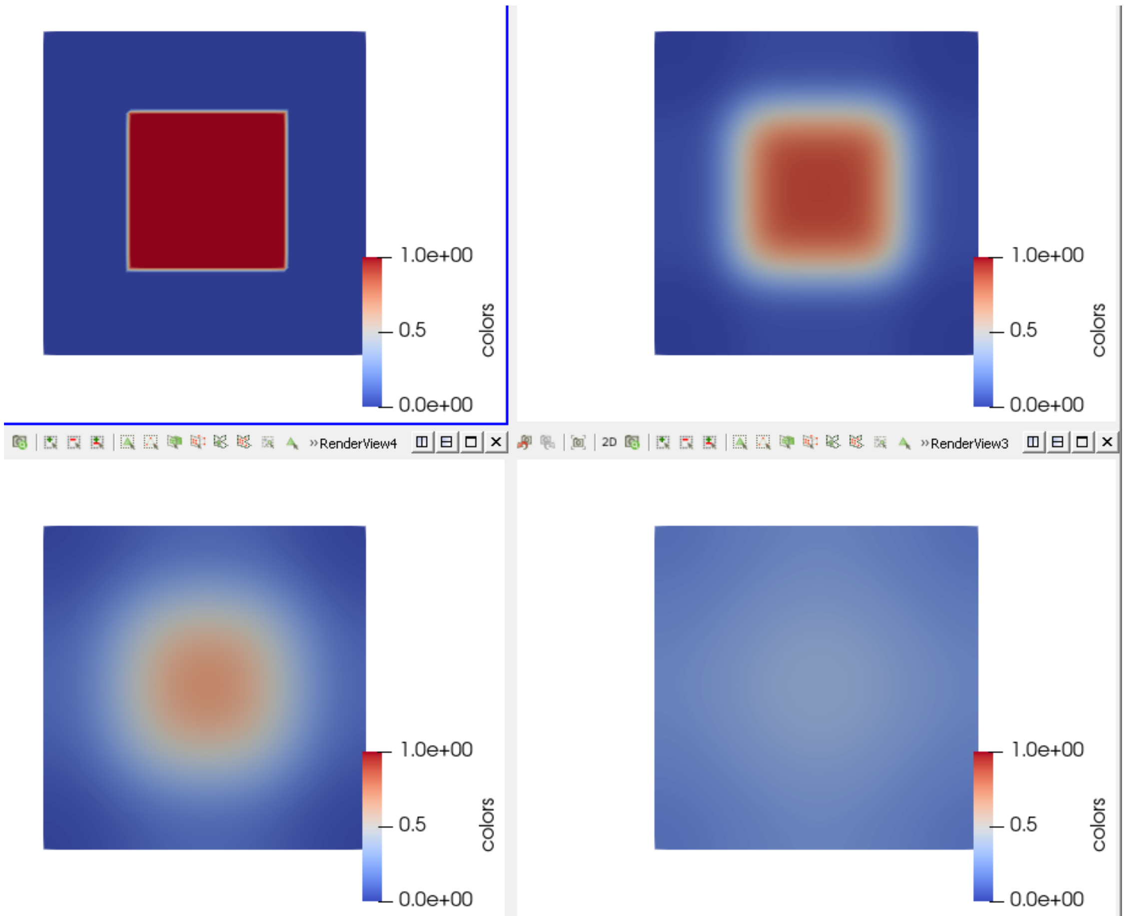
Комп'ютерне моделювання задач прикладної математики

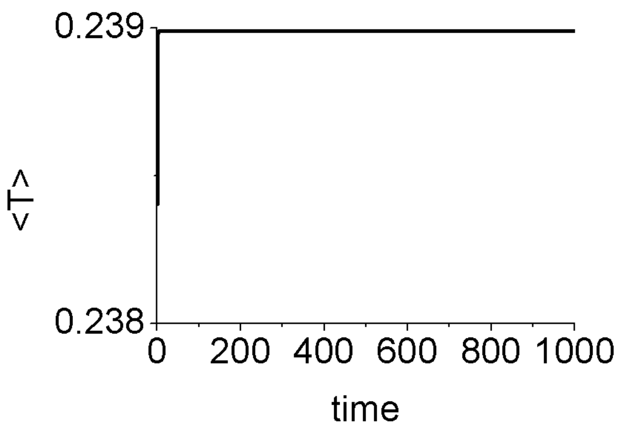
Реакційно-дифузійні системи та їх застосування

Лекція 15

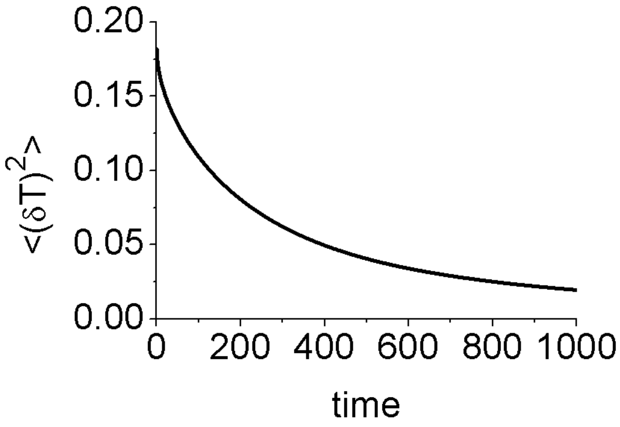
Звичайне рівняння дифузії

$$\frac{\partial T(\mathbf{r},t)}{\partial t} = \nabla^2 T$$



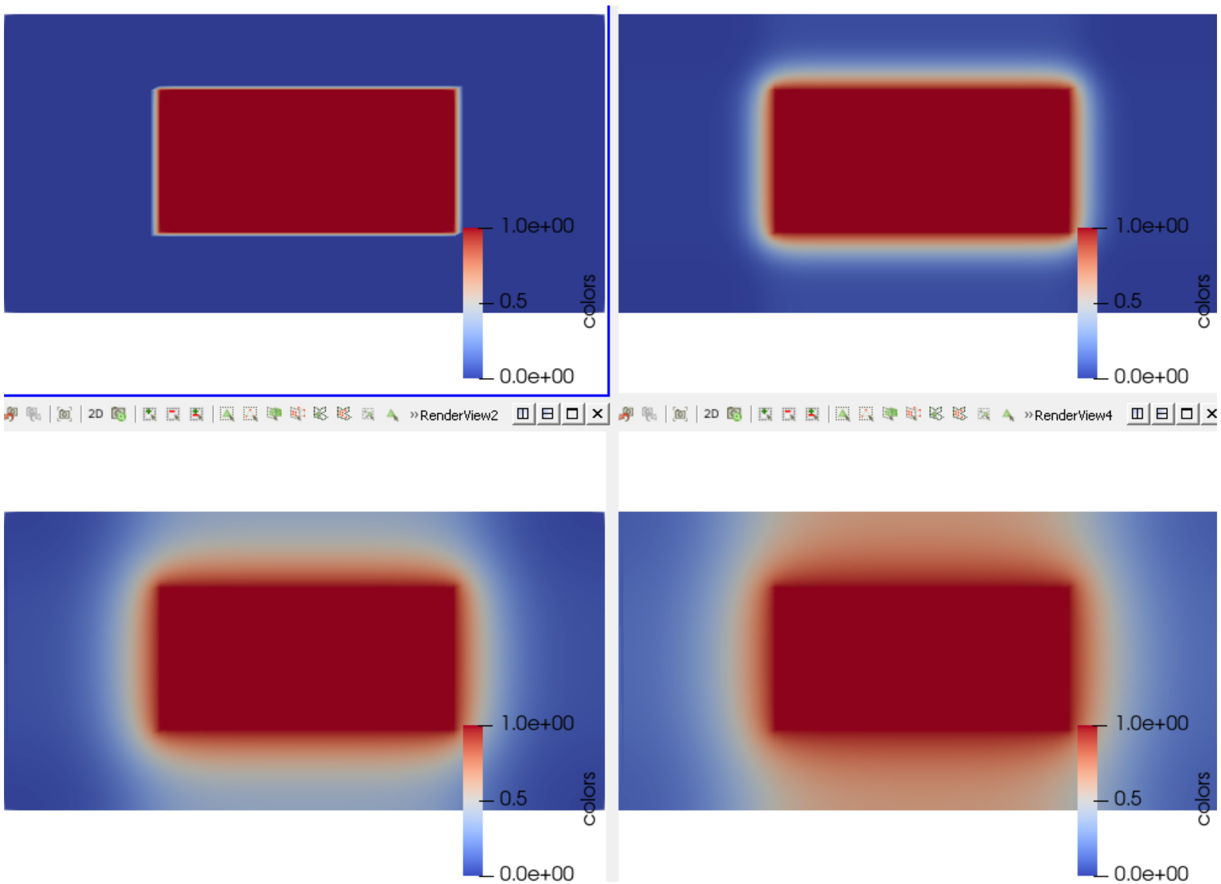


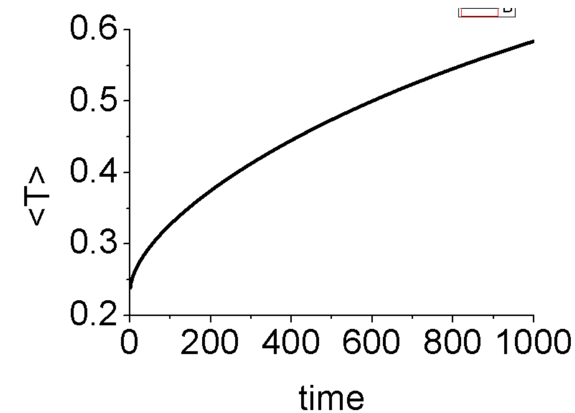
$$\langle(\delta T)^2\rangle = \langle T^2\rangle - \langle T\rangle^2$$



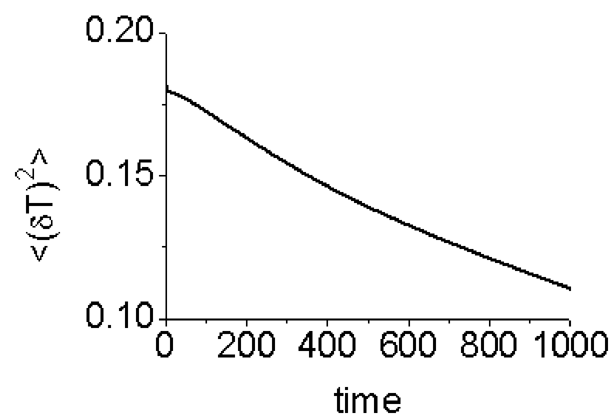
Звичайне рівняння дифузії

$$\frac{\partial T(\mathbf{r},t)}{\partial t} = \nabla^2 T + W(\mathbf{r})$$



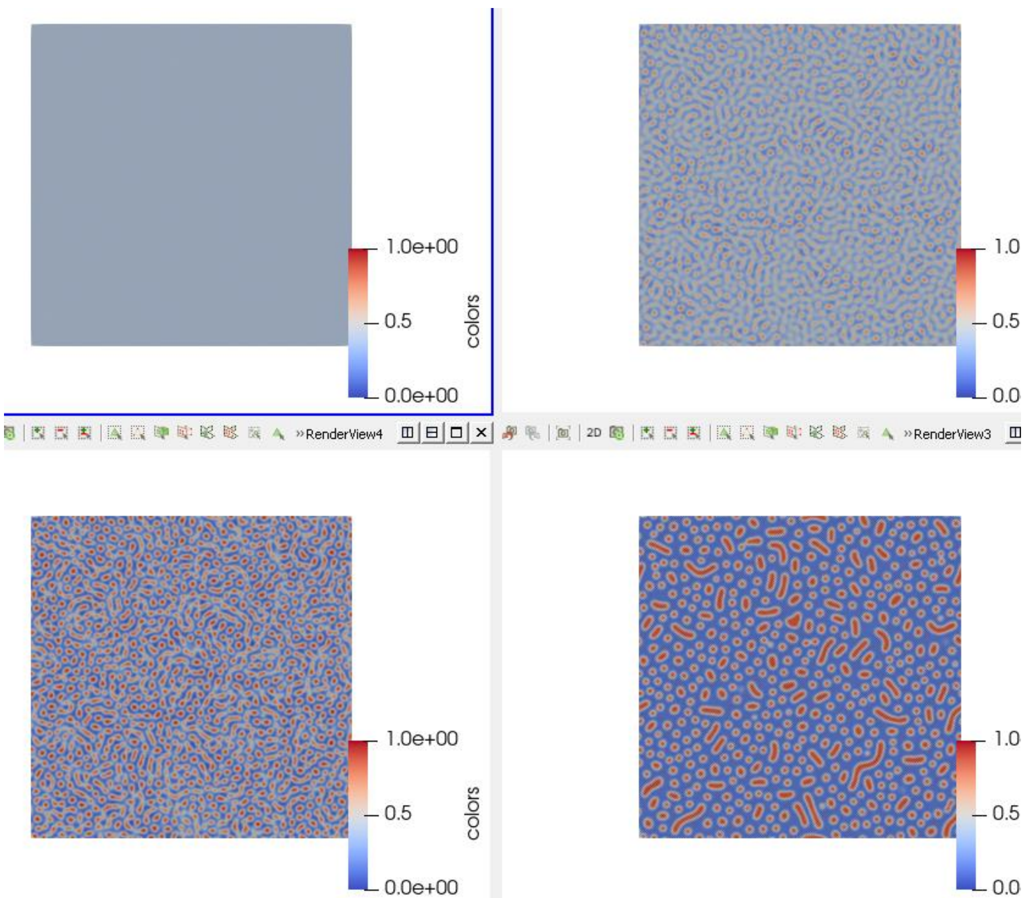


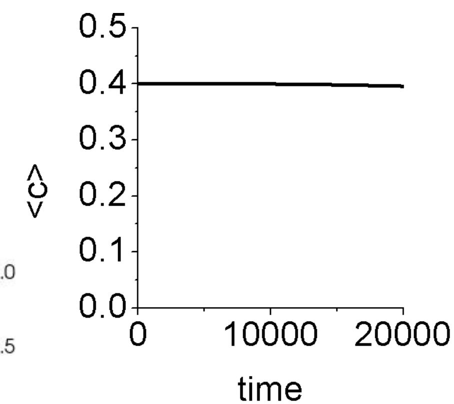
$$\langle(\delta T)^2\rangle = \langle T^2\rangle - \langle T\rangle^2$$

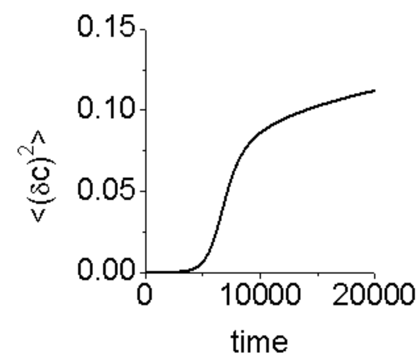


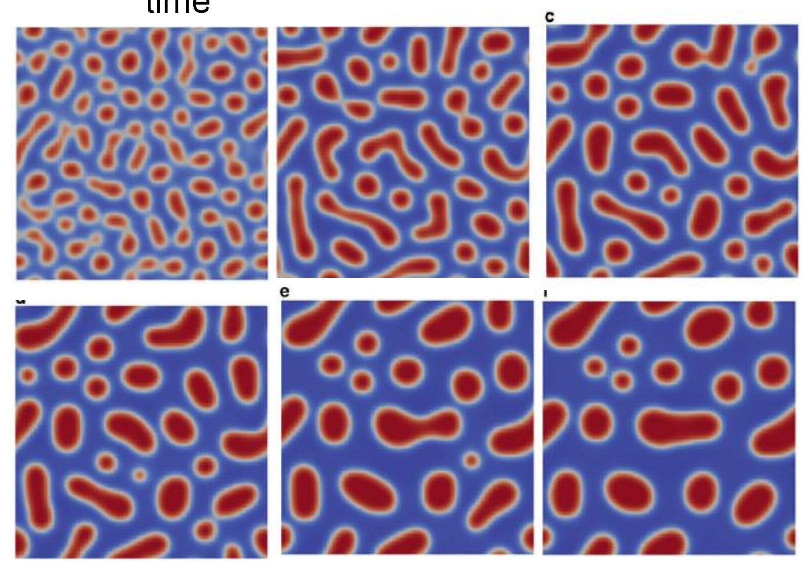
Модель фазового розшарування

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = \nabla^2\left[-c + c^3 - \kappa\nabla^2 c\right]$$









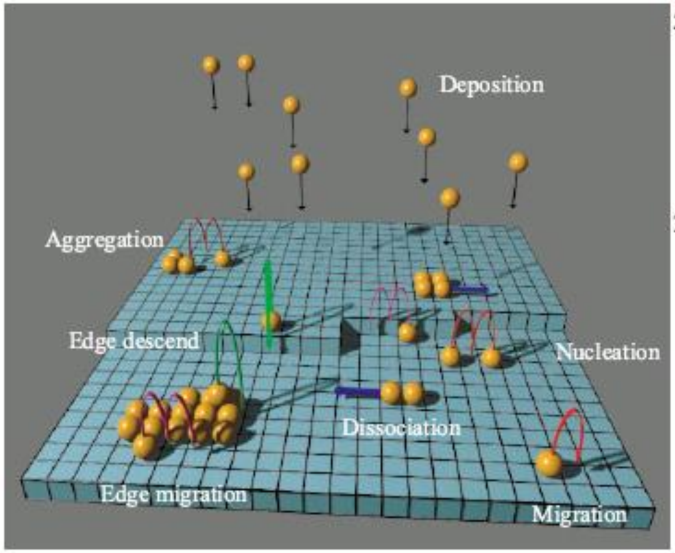
Реакційно-дифузійні рівняння

$$\frac{\partial \phi(\mathbf{r},t)}{\partial t} = \nabla \cdot \left[M(\phi) \nabla \frac{\delta F[\phi(\mathbf{r},t)]}{\delta \phi(\mathbf{r},t)} \right] + f(\phi)$$

$$F = \int_V \left[F_0(\phi) + \frac{1}{2} \kappa (\nabla \phi)^2 \right] dV$$

$$\frac{\partial \phi(\mathbf{r},t)}{\partial t} = f(\phi) + \nabla \cdot \left[M(\phi) \nabla \left\{ \frac{dF_0}{d\phi} - \kappa \nabla^2 \phi \right\} \right]$$

Формування структур адсорбату на поверхнях тонких плівок



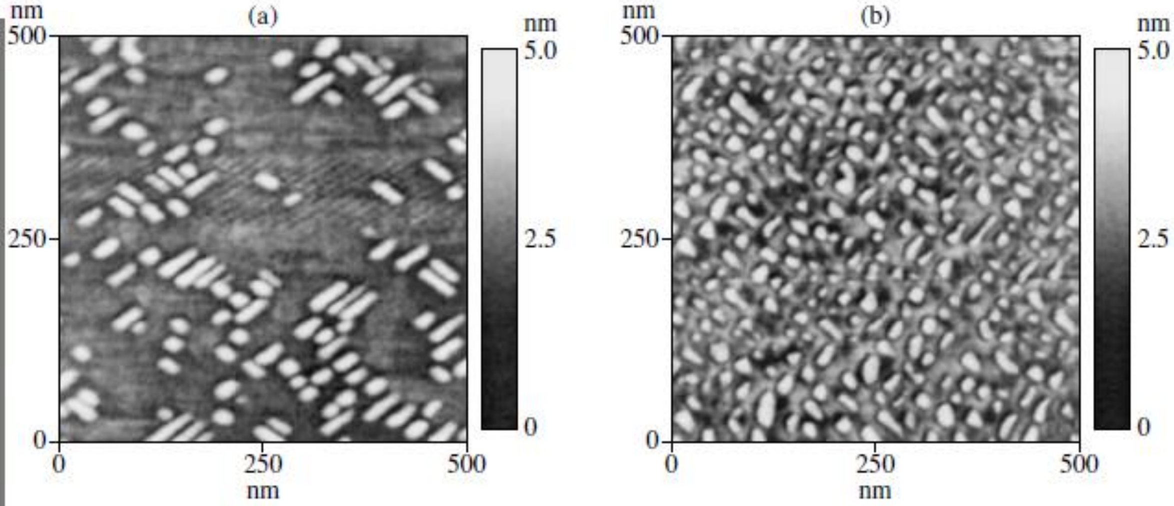
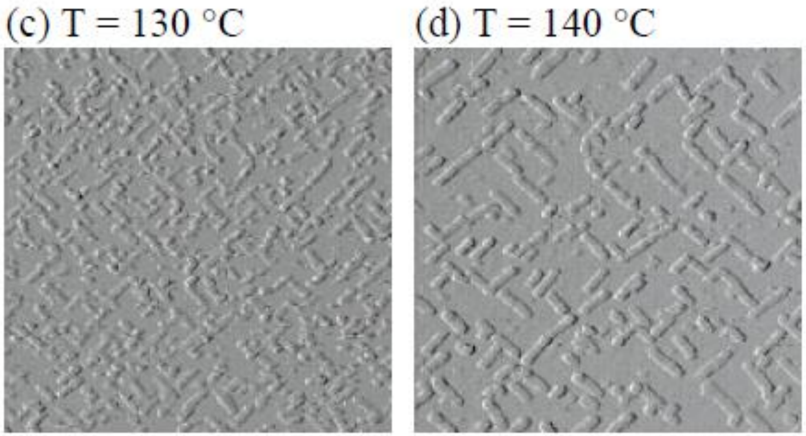
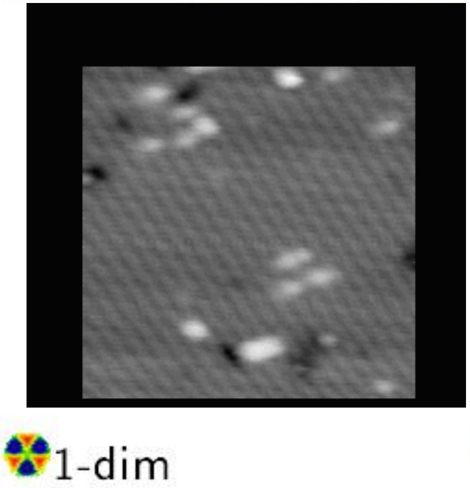
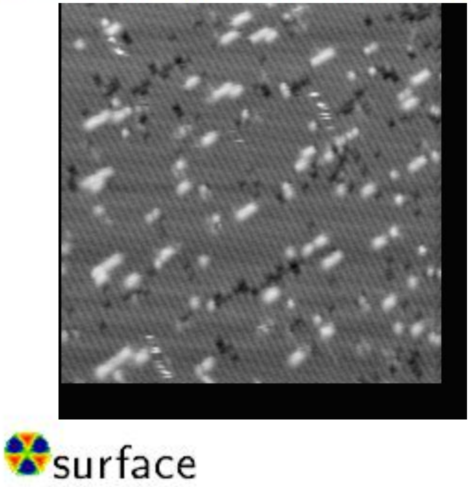


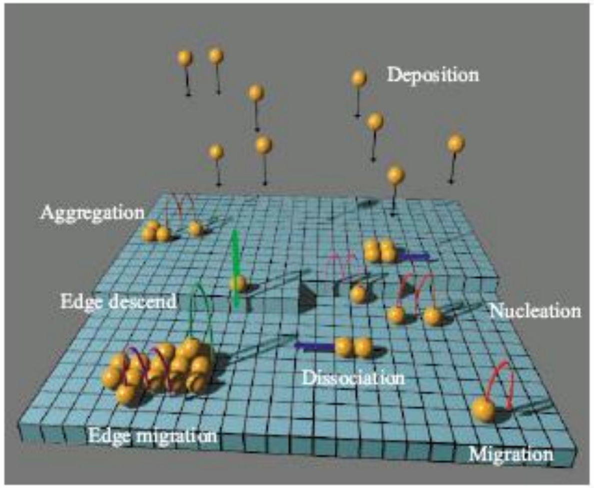
Fig. 3. Surface AFM image of a structure with a GeSi sublayer after the deposition of (a) 7 Å of Ge and (b) 9 Å of Ge.







Формування структур адсорбату на поверхнях тонких плівок



Adsorption-desorption systems [M.Hildebrand, A.S.Mikhailov, J.Phys.Chem.,1996]

Equilibrium chemical reactions: $f(x) = adsorption + desorption$

- adsorption term: $k_a p(1-x)$
- desorption term: $-k_d x$, $k_d = k_{d0}\exp(U(r)/T)$

Total flux: $\mathbf{J} = \mathbf{J}_D + \mathbf{J}a$

- Stationary diffusion flux: $\mathbf{J}_D = -D_0 \nabla x$
- Stationary flow of adsorbate $\mathbf{J}_a = \mathbf{v}x = (D_0/T)\cdot\mathbf{F}x = -(D_0/T)x(1-x)\nabla U$

Формування структур адсорбату на поверхнях тонких плівок

The local coverage at surface: $x(\mathbf{r},t) \in [0,1]$.
The reaction term :

$$f_0(x) = k_a p(1-x) - k_d x \exp(U(\mathbf{r})/T) - k_r x^2$$

The total stationary flux

$$\mathbf{J} = -D_0 M(x) \nabla \frac{\delta \mathcal{F}}{\delta x}, \quad \mathcal{F} = \mathcal{F}_0 + \mathcal{F}_{int}; \quad M(x) = x(1-x). \tag{1}$$

Free energy components

$$\mathcal{F}_0 = \int \mathrm{d}\mathbf{r} \left[x \ln(x) + (1-x)\ln(1-x) \right], \quad F_{int} = \frac{1}{T} \int \mathrm{d}\mathbf{r} x U \tag{2}$$

The interaction potential is

$$\frac{U(\mathbf{r})}{T} = -\frac{1}{T} \int \mathrm{d}\mathbf{r}' u(\mathbf{r}-\mathbf{r}')x(\mathbf{r}') \simeq -\varepsilon(1+\rho_0^2\nabla^2)^2 x, \quad \varepsilon \equiv \frac{u(0)}{T} \tag{3}$$

Формування структур адсорбату на поверхнях тонких плівок

$$\partial_t x = f(x) - \nabla \cdot \mathbf{J}; \quad \mathbf{J} = -M(x)\nabla \frac{\delta \mathcal{F}}{\delta x}, \tag{4}$$

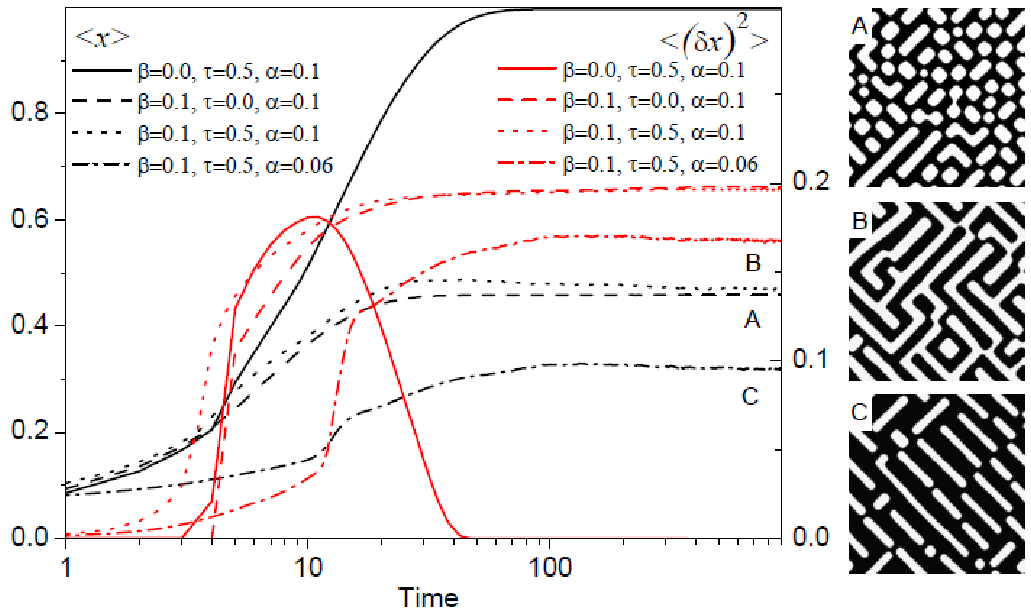
$$f(x) = \alpha(1-x) - xe^{-2\varepsilon x} - \beta x^2, \quad M(x) = x(1-x) \tag{5}$$

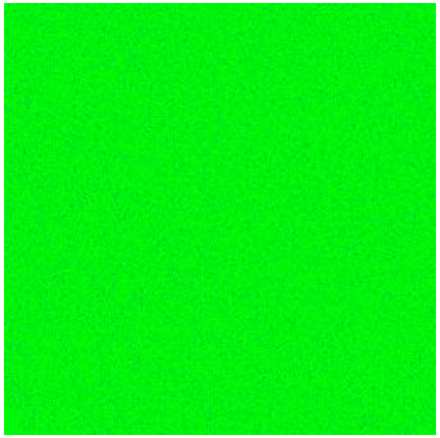
Deterministic equation

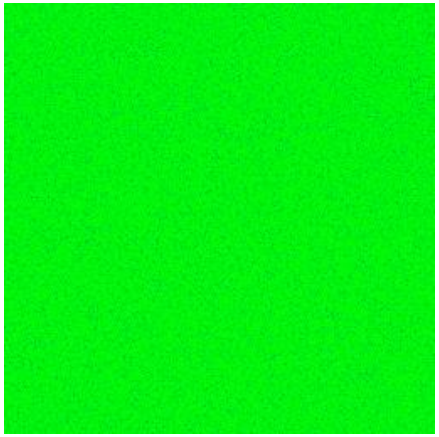
$$\partial_t x = \varphi(x; \nabla), \tag{6}$$

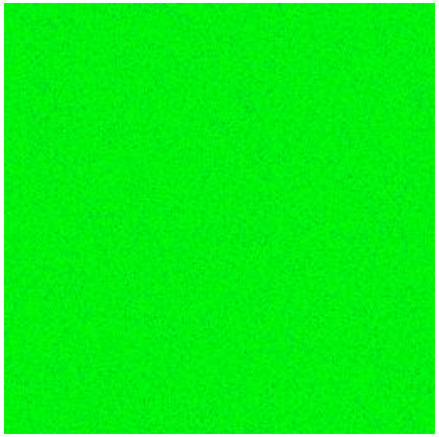
$$\varphi(x; \nabla) \equiv f(x) + \nabla \cdot [\nabla x - \varepsilon M(x)(\nabla x + \nabla(1 + \rho_0^2 \nabla^2)^2 x)]. \tag{7}$$

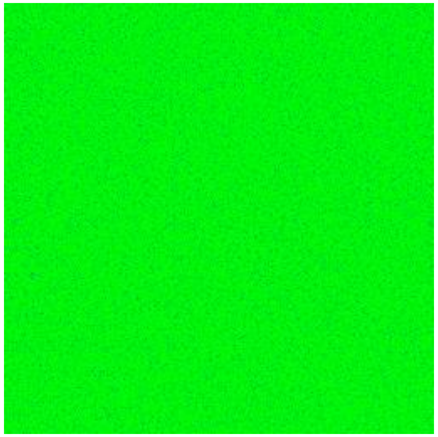
Формування структур адсорбату на поверхнях тонких плівок



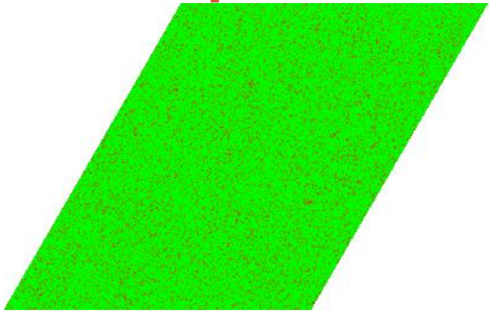


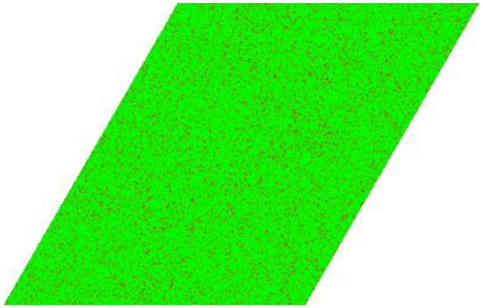


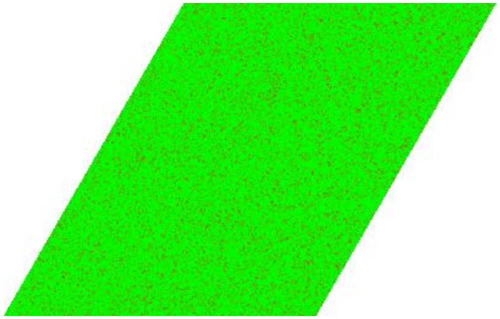


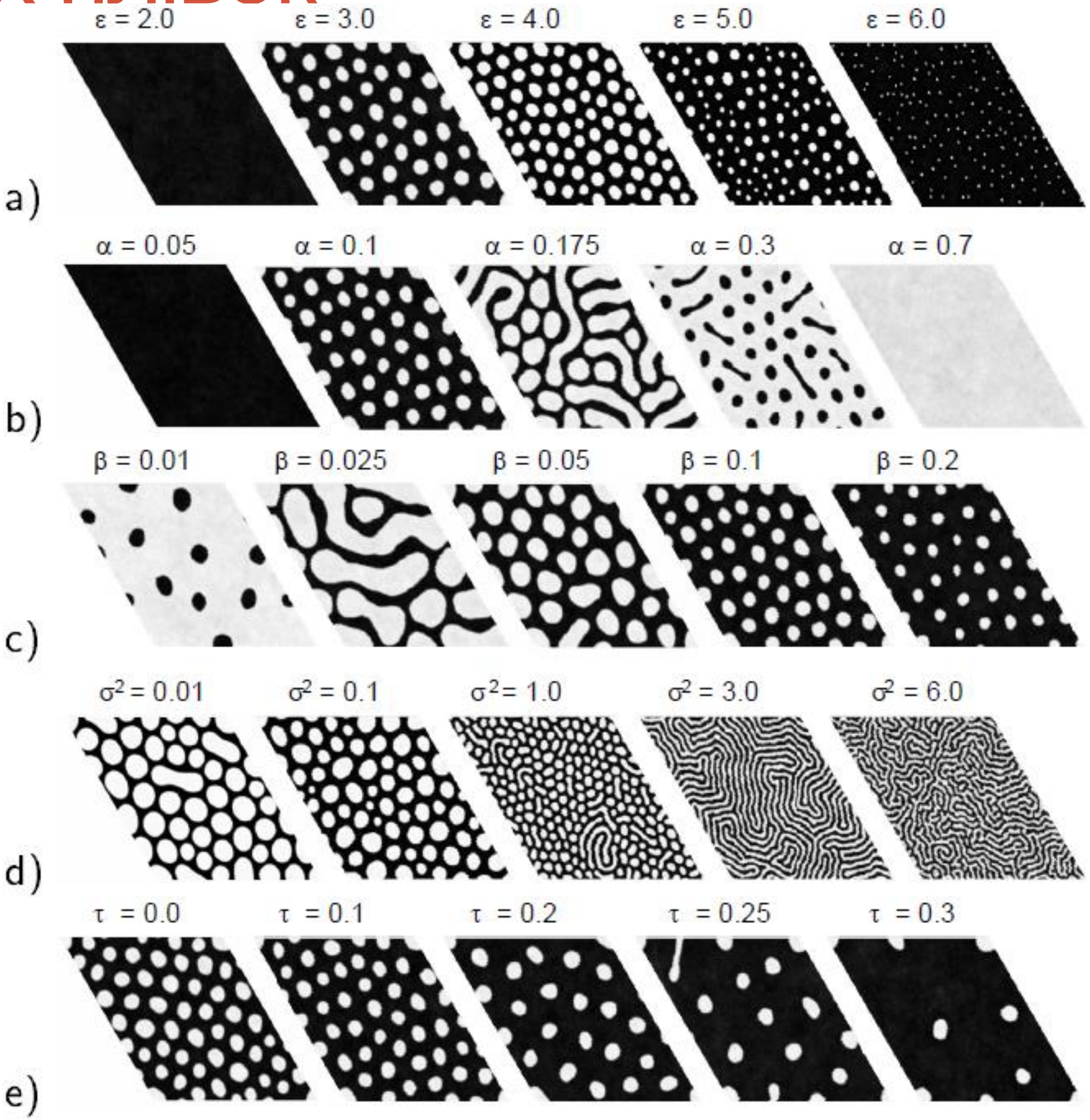


Формування структур адсорбату на поверхнях тонких плівок

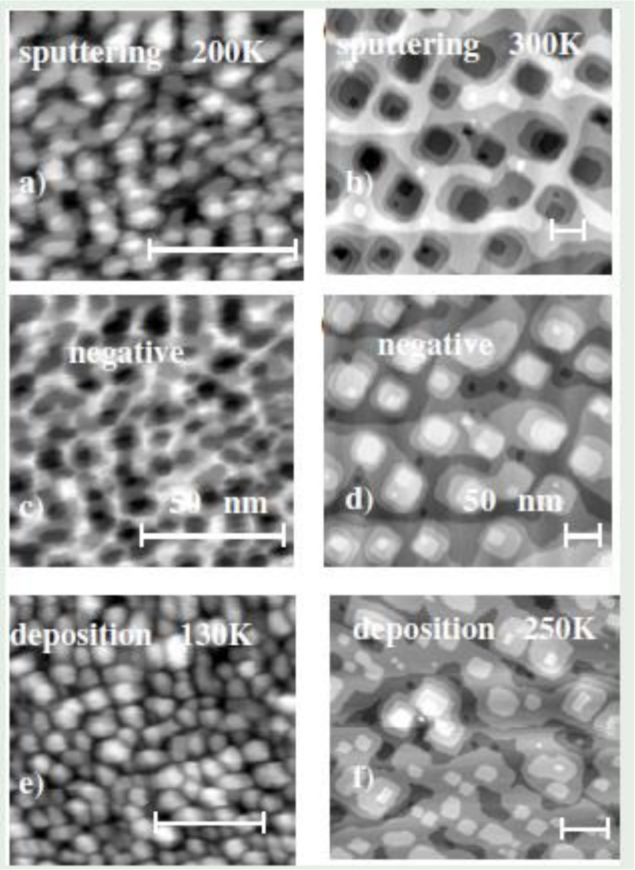


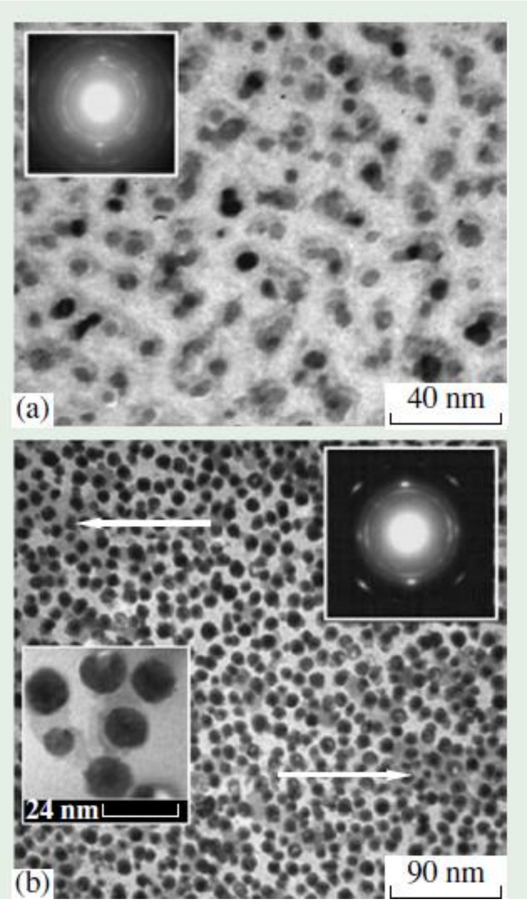




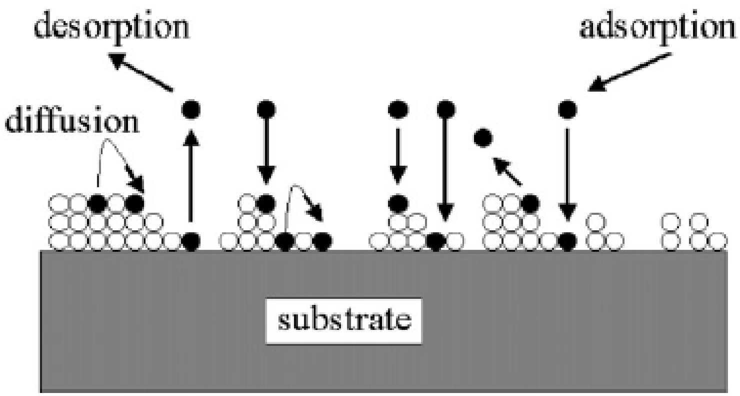


Багатошарові структури





Багатошарові структури



- $c_i(\mathbf{r}, t)$ is the local coverage in the i-th layer (monoatomic level)
- $f_i(\{c_i(\mathbf{r}, t)\}_{i=1}^n)$ is the reaction term
- $\mathbf{J}_i(\{c_i(\mathbf{r}, t)\}_{i=1}^n, \nabla)$ is the diffusion flux
- Vectors:

$$\vec{c}(\mathbf{r}, t) = \{c_i(\mathbf{r}, t)\}_{i=1}^n;$$

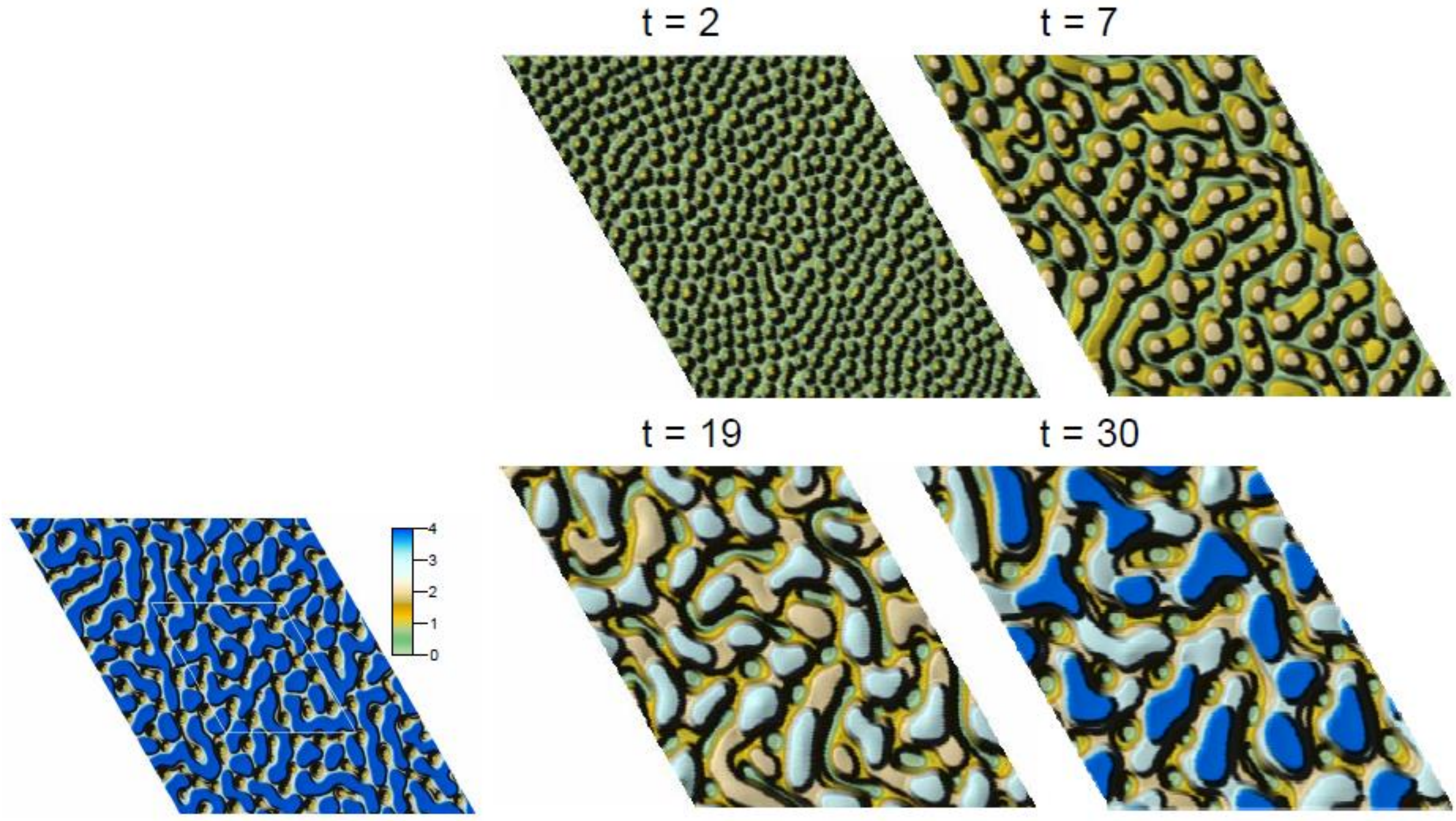
$$\vec{f}(\vec{c}(\mathbf{r}, t)) = \{f_i(\vec{c}(\mathbf{r}, t))\}_{i=1}^n;$$

$$\vec{\mathbf{J}}(\vec{c}(\mathbf{r}, t), \nabla) = \{\mathbf{J}_i(\vec{c}(\mathbf{r}, t), \nabla)\}_{i=1}^n$$

The generalized model for the adsorptive multilayer system:

$$\partial_t \vec{c}(\mathbf{r}, t)) = \vec{f}(\vec{c}(\mathbf{r}, t)) - \nabla \cdot \vec{\mathbf{J}}(\vec{c}(\mathbf{r}, t), \nabla).$$

Багатошарові структури



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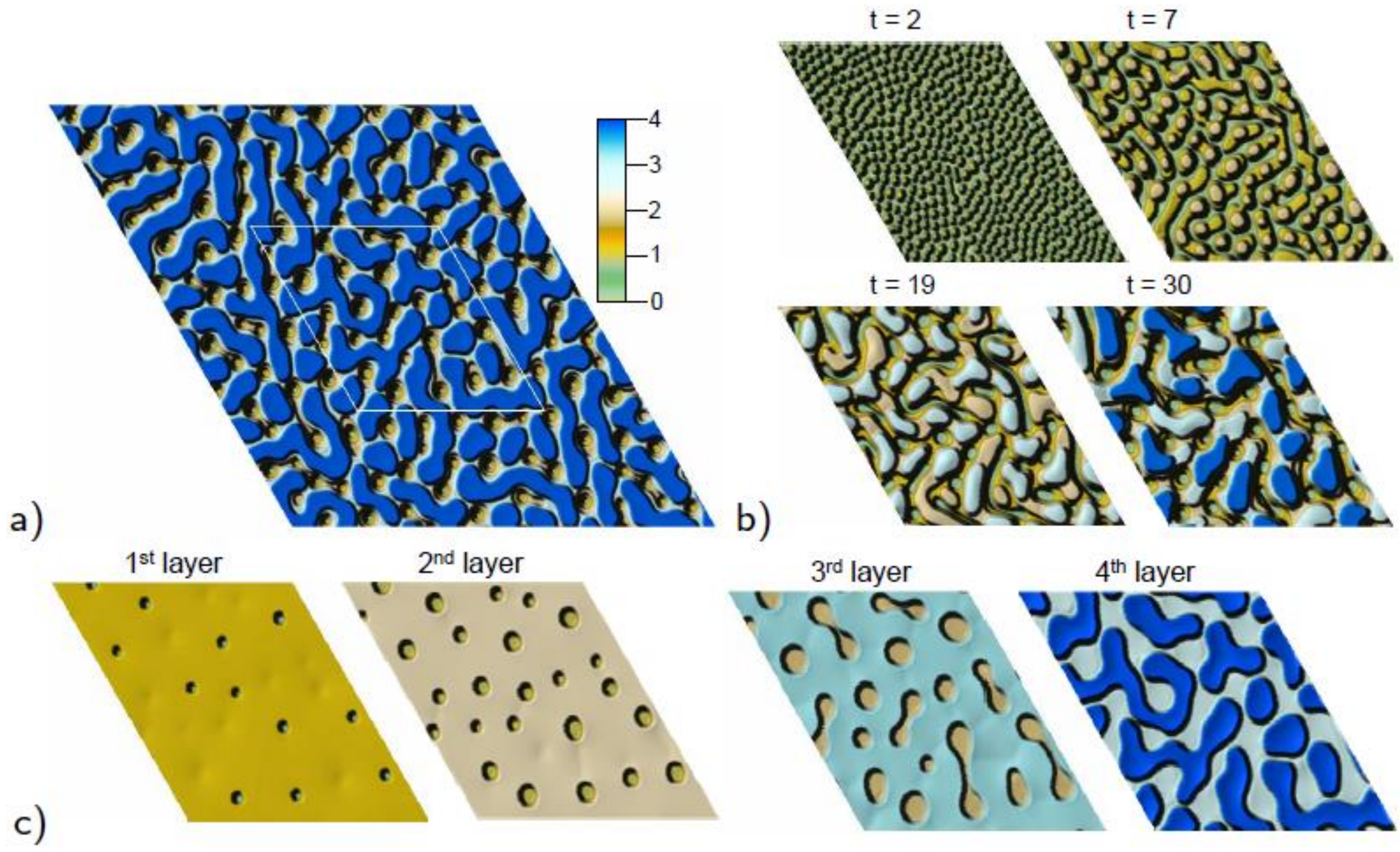

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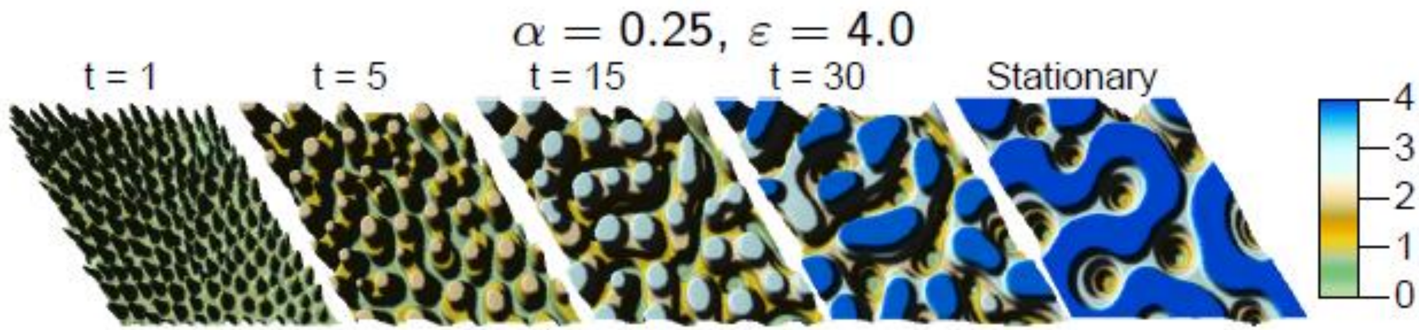
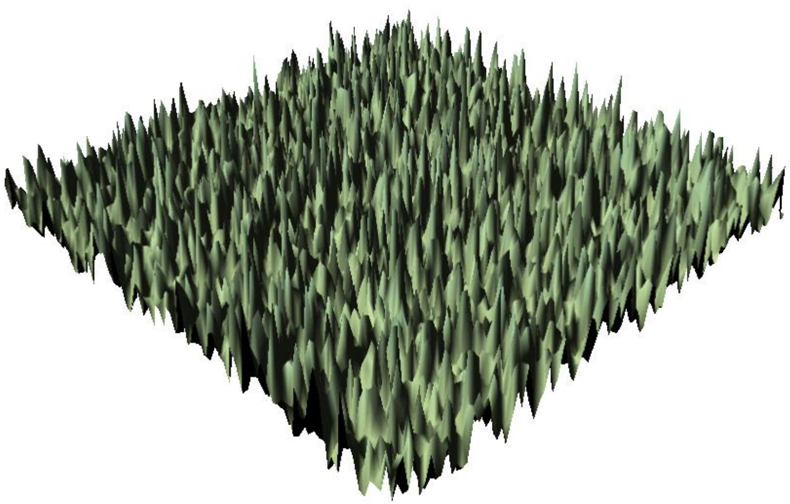
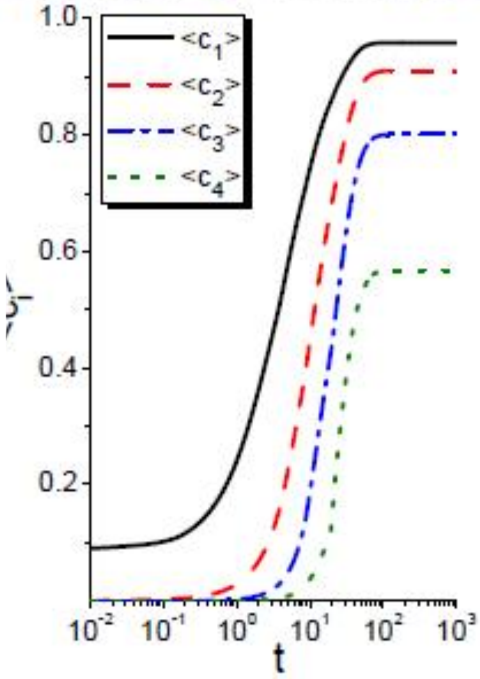
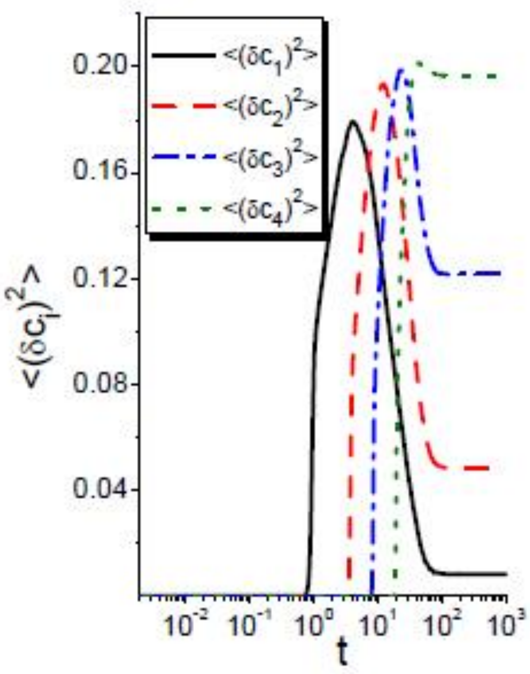




Evolution





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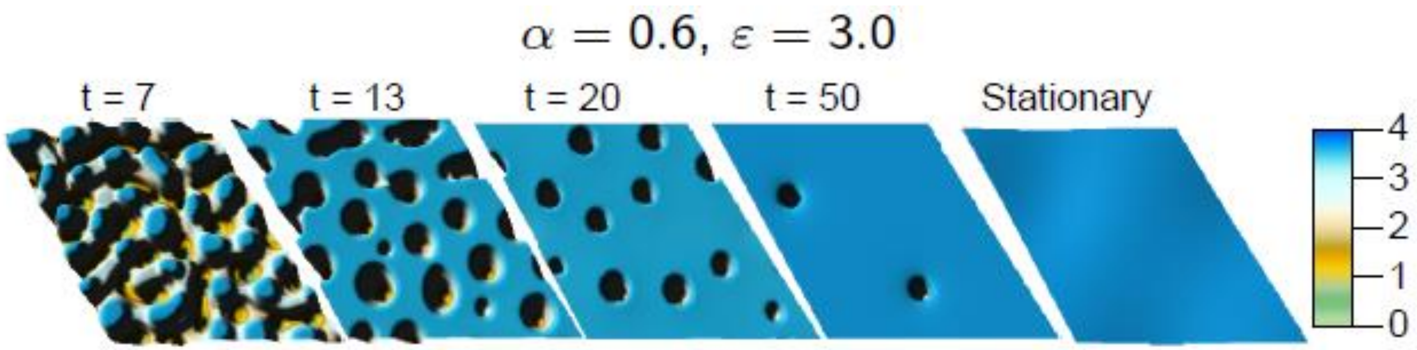
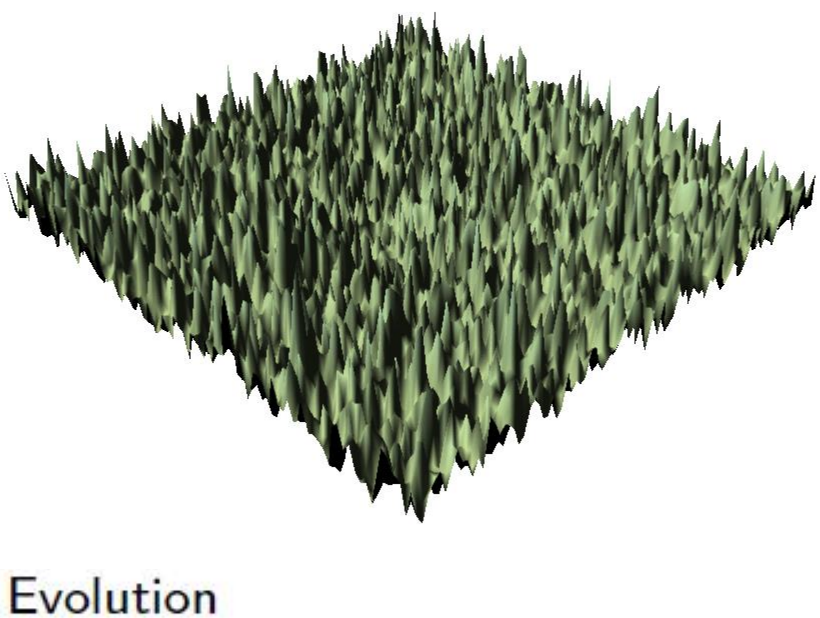
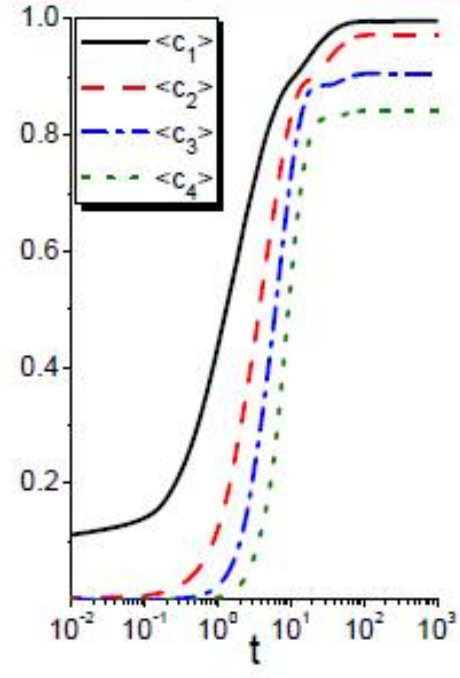
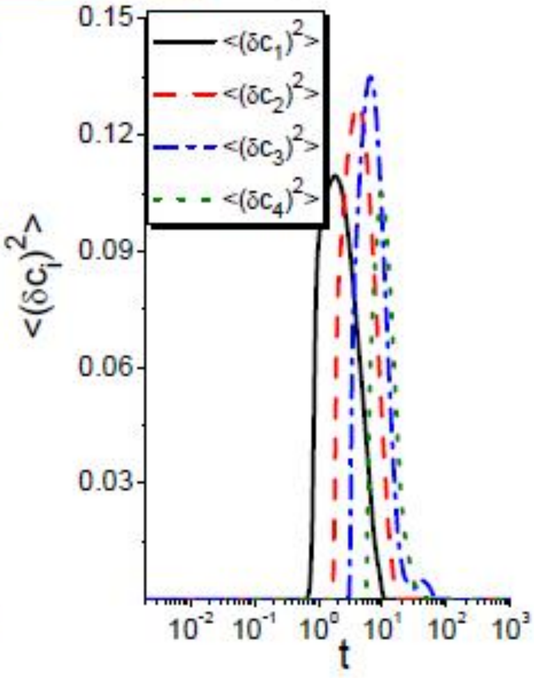


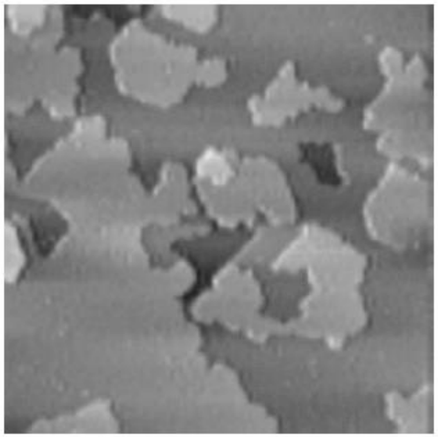


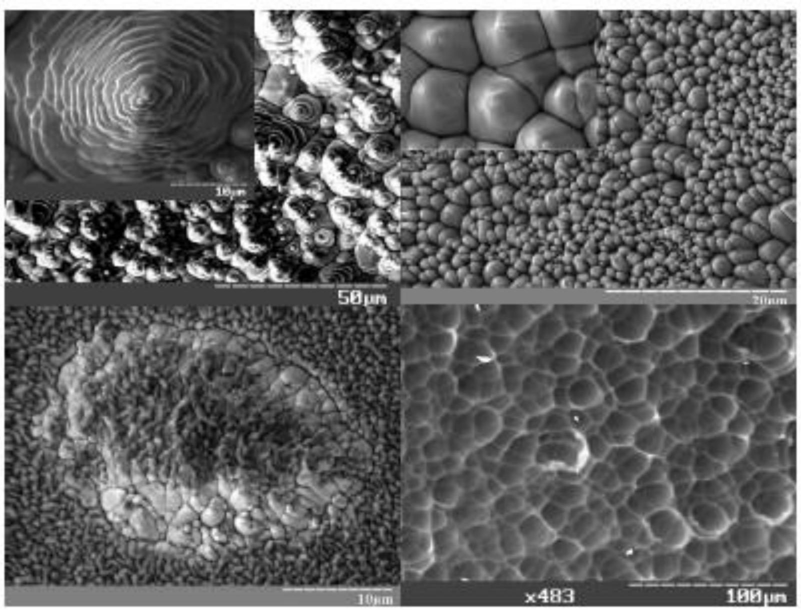


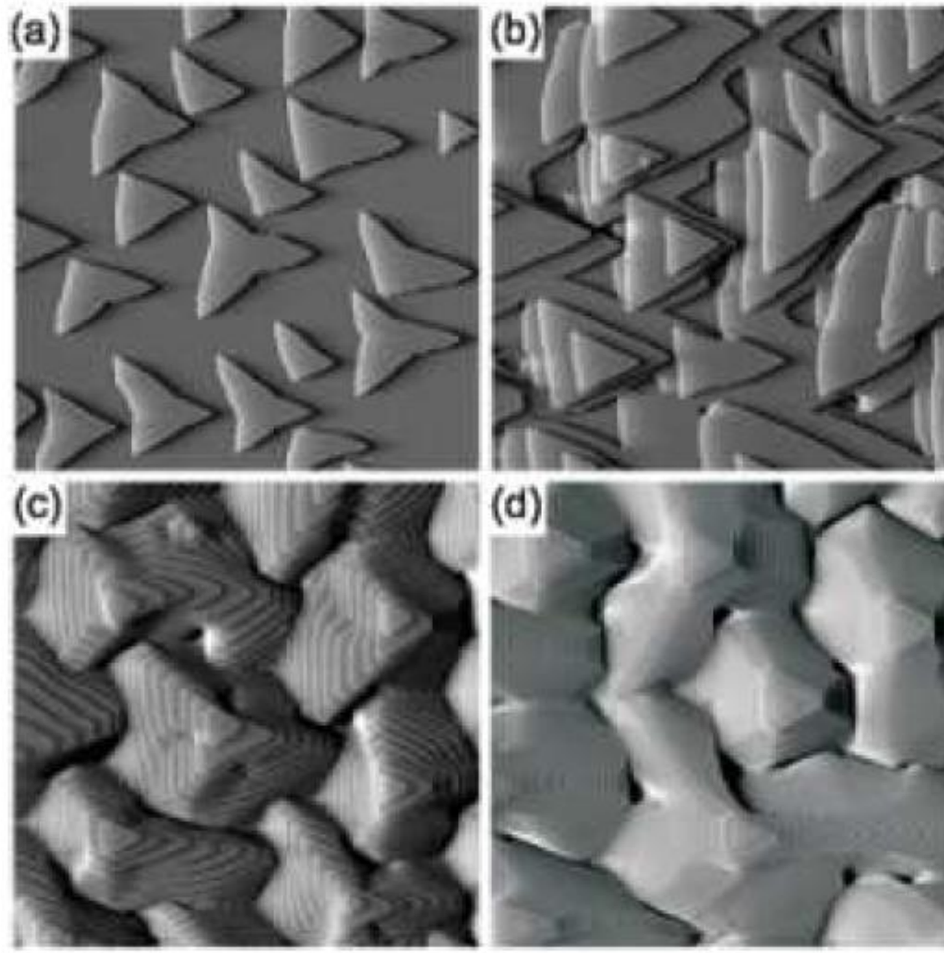


Пірамідальні структури

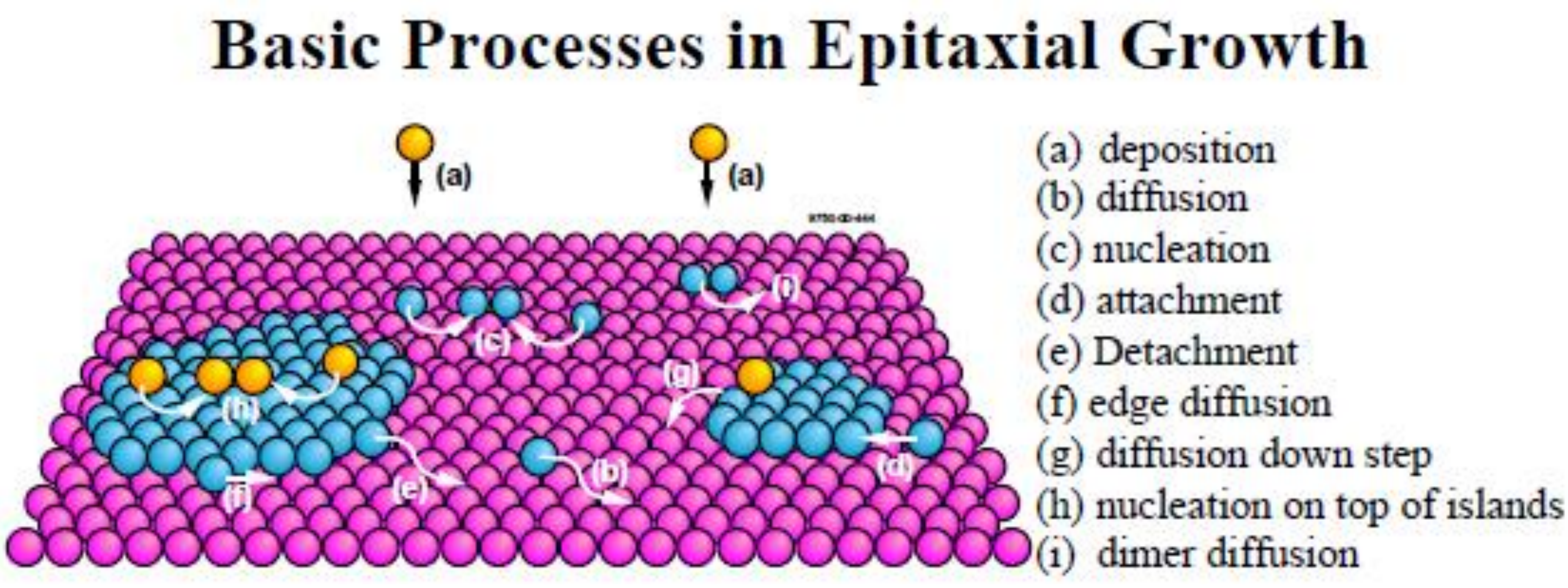
Пірамідальні структури







Пірамідальні структури



Пірамідальні структури

$$\frac{\partial x}{\partial t} = F - \frac{x}{\tau_x} - \nabla \cdot \mathbf{J}_{tot}.$$

$$\partial_t x = F - \frac{x}{\tau_{x0}} e^{U/T} - \nabla \cdot \mathbf{J}_{tot}; \quad \mathbf{J}_{tot} = -D\left[\nabla x + x(1-x)\nabla(U/T)\right].$$

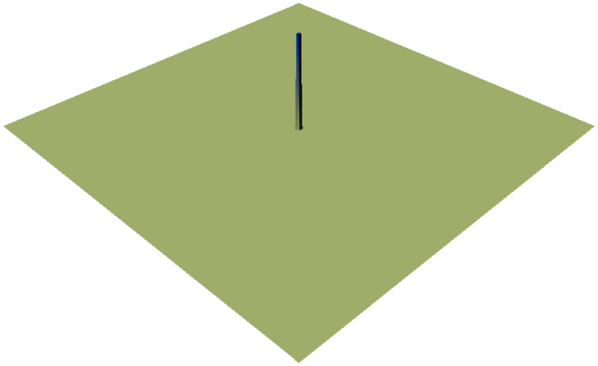
$$\partial_t x = F_0 - \frac{x}{\tau_{x0}} e^{U/T} - \nabla \cdot \mathbf{J}_{tot} - \frac{1}{2}\partial_t \phi;$$

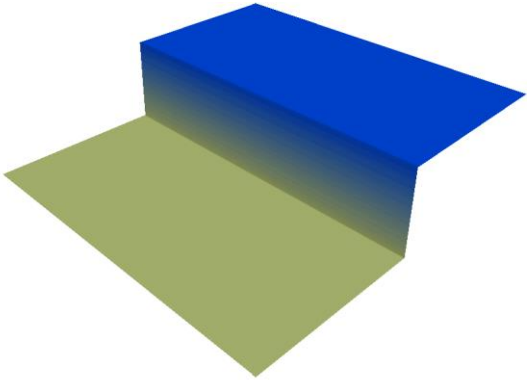
$$\tau_\phi \partial_t \phi = -\frac{\delta H}{\delta \phi}.$$

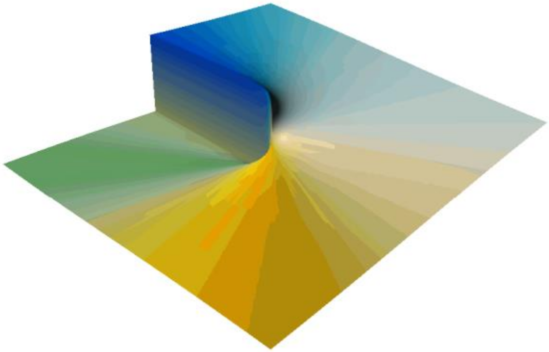
$$\tau_\phi \partial_t \phi = -\frac{\delta H}{\delta \phi},$$

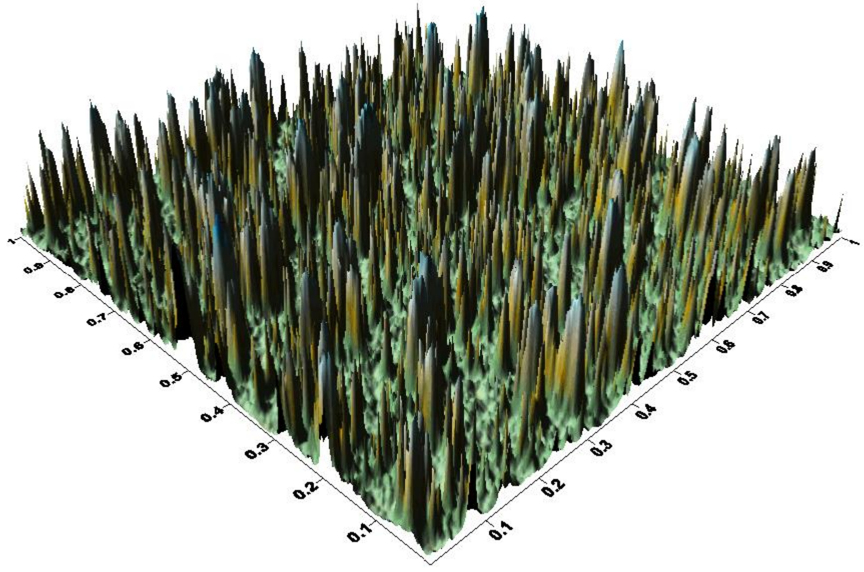
$$H = \int \mathrm{d}\mathbf{r} \left[\frac{\varpi^2}{2}(\nabla\phi)^2 + \frac{1}{2\pi}\cos(2\pi[\phi - \phi_s]) - \lambda x \left(\phi + \frac{1}{2\pi}\sin(2\pi[\phi - \phi_s])\right)\right]$$

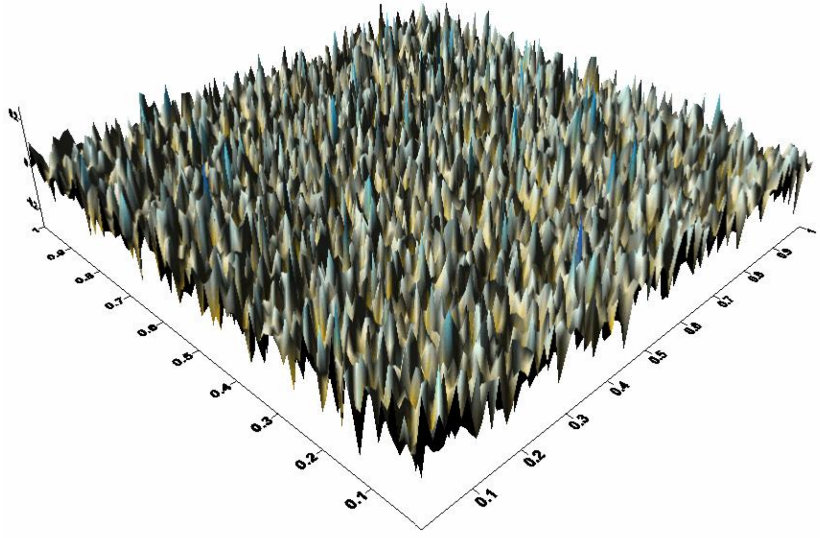
Пірамідальні структури











Еволюція поверхні при розпорошенні

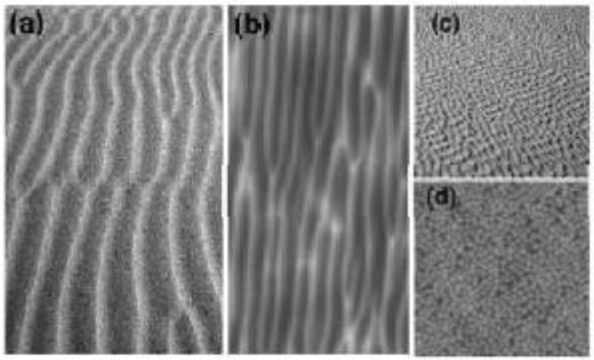


Fig. 1. (a) Ripples on a sand dune in Morocco. Photograph courtesy of J. Rodríguez and E. Blesa. (b) $3.7 \times 6.7\ \mu m^2$ top view AFM image of a Si surface immersed in argon plasma. (c) "Dots" on a sand dune in New Mexico, USA. Copyright Bruce Molnia, Terra Photographics. Image Courtesy Earth Science World Image Bank http://www.earthscienceworld.org/images. (d) $1 \times 1\ \mu m^2$ top view AFM image of a GaSb surface irradiated by 0.7 keV Ar^+ ions under normal incidence.

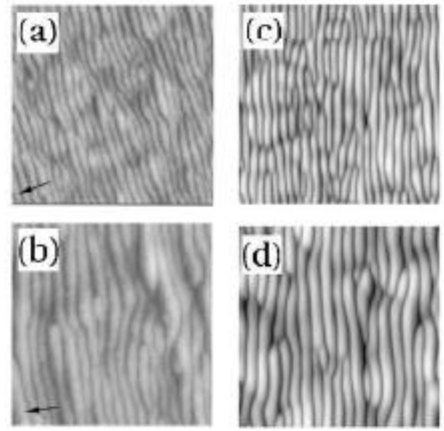
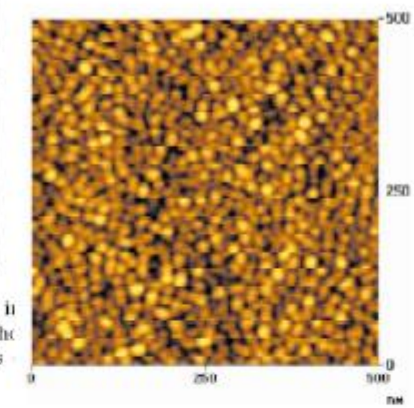


Fig. 26. (a), (b) $1 \times 1\ \mu m^2$ AFM views of fused silica targets i oblique incidence after 10 and 60 min, respectively; (c), (d) morphc by numerical integration of Eq. (26) at times t_1 and $6t_1$. Panels taken from [63] with permission.

ION-INDUCED PATTERN FORMATION ON Co . . .



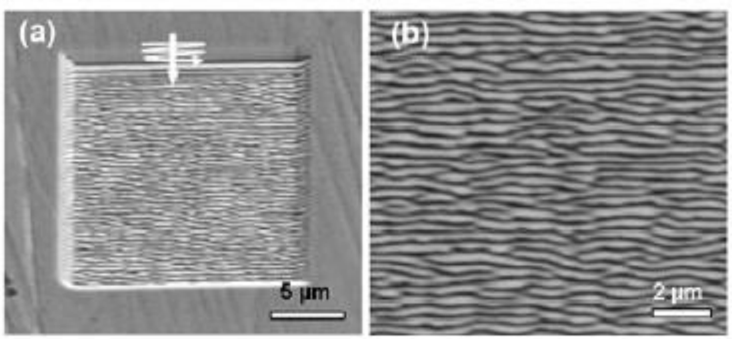
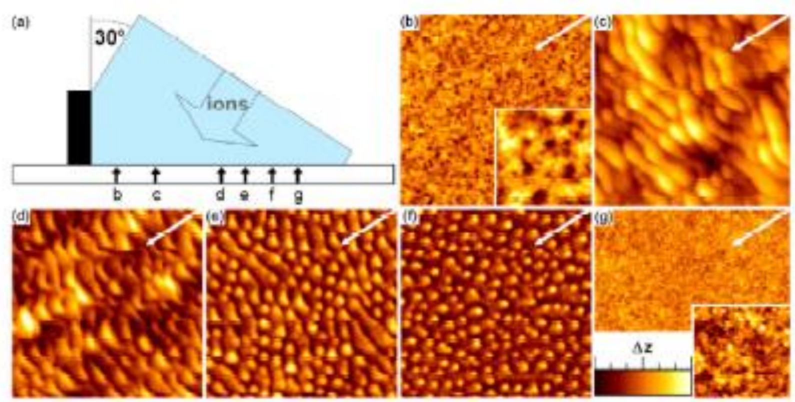
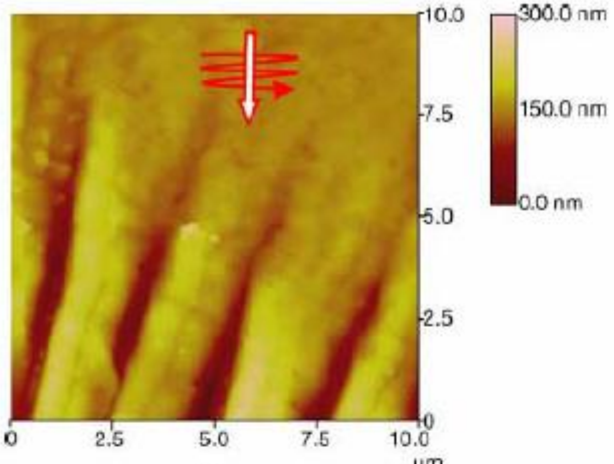


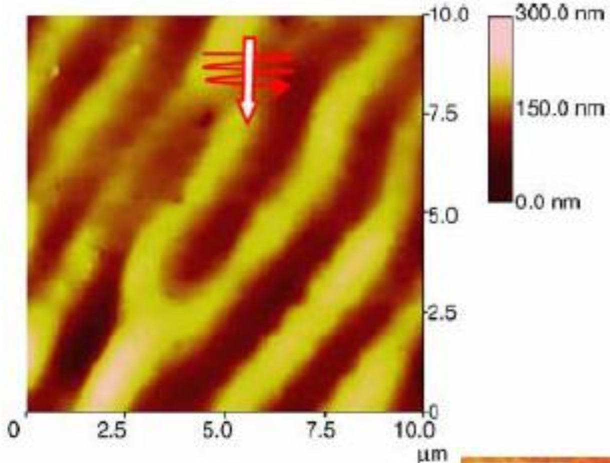
FIG. 1. (a) A SEM image showing the ripples created by 30 keV Ga^+ focused ion beam bombardment on a $Cd_2Nb_2O_7$ single crystal surface (ion current, 0.3 nA; incident angle, 50°; patterned area, $15 \times 10\ \mu m^2$; and ion fluence of 5.38×10^{17} ions/cm^2). The orientation of the ripples is perpen-



Еволюція поверхні при розпорошенні



(a)



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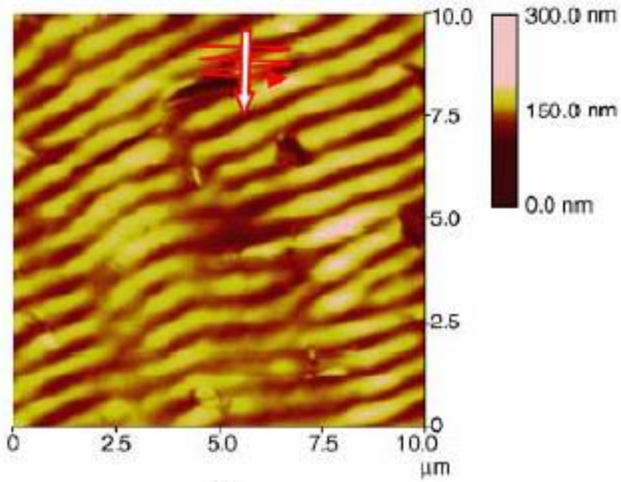

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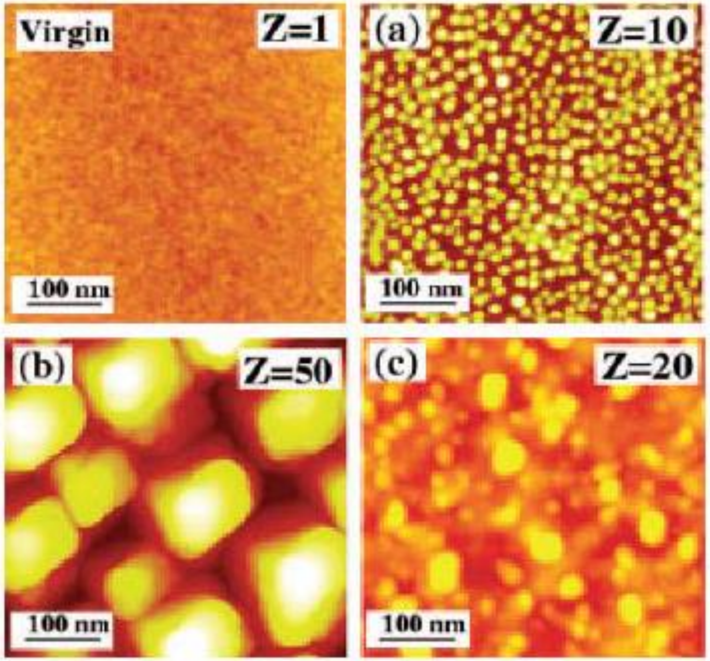

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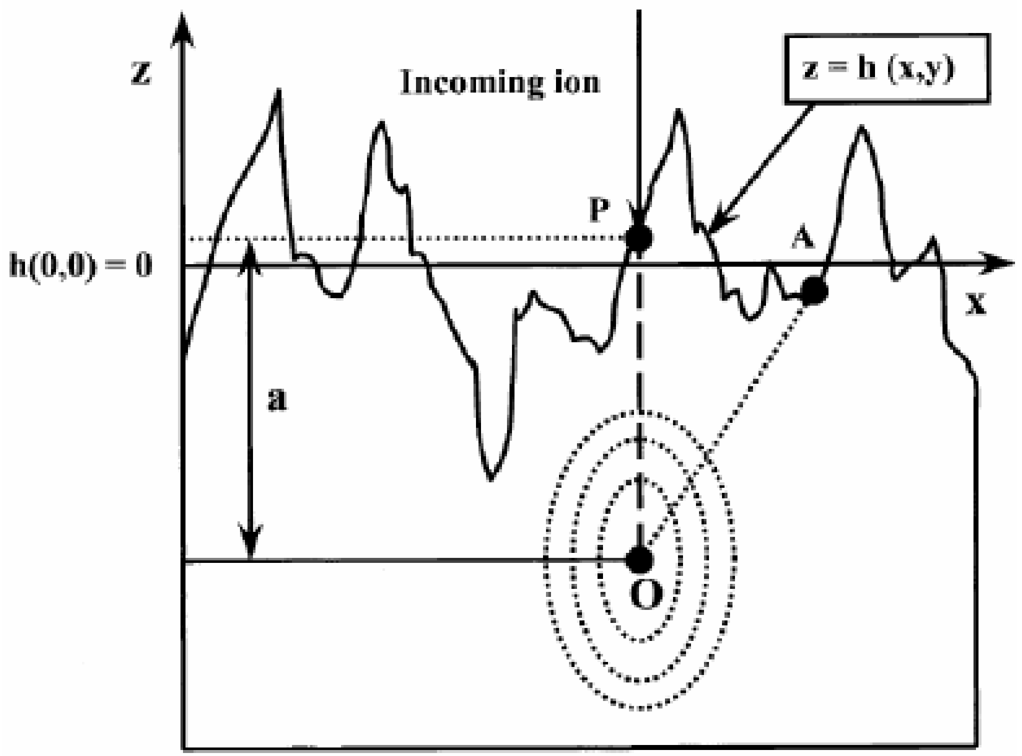
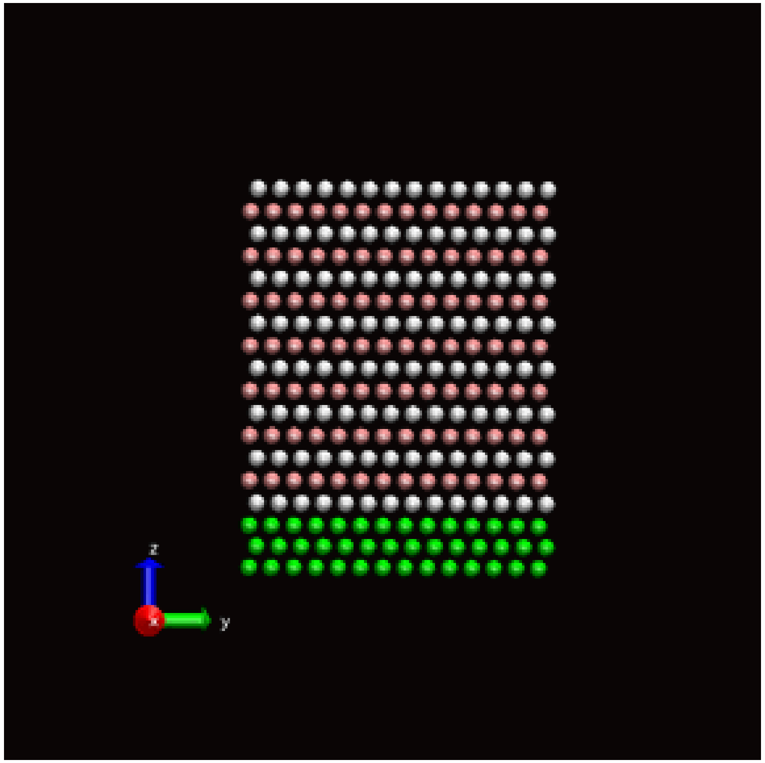




Еволюція поверхні при розпорошенні

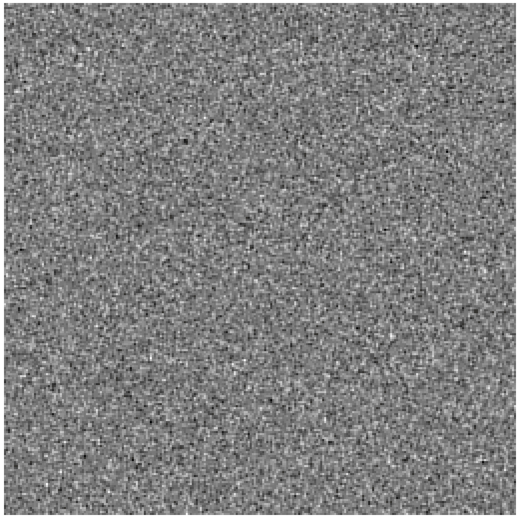
Evolution equation of the height field

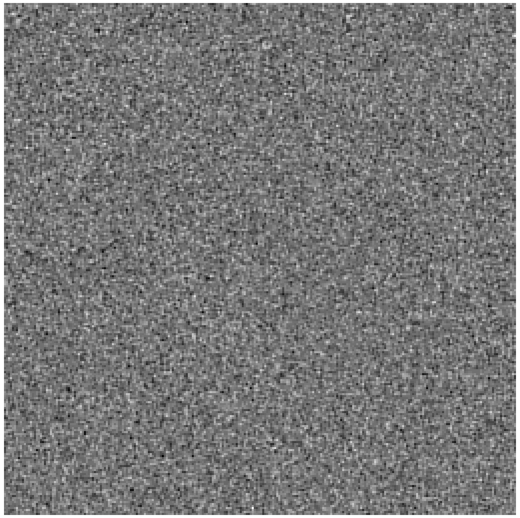
$$\partial_t h \simeq -v(\theta - \nabla_x h, \nabla_x^2 h, \nabla_y^2 h) - \nabla \cdot \mathbf{j}_s.$$

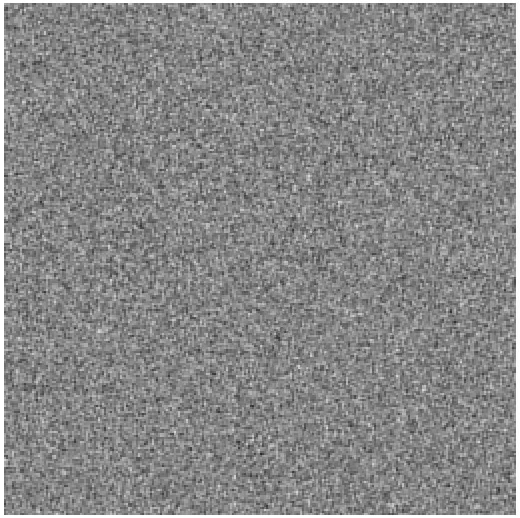
The surface current

$$\mathbf{j}_s = K\nabla(\nabla^2 h); \quad K = D_s \kappa \rho / n^2 T, \quad D_s = D_0 e^{-E_a/T}$$

$$\partial_t h = \gamma \nabla_x h + \nu_\alpha \nabla^2_{\alpha\alpha} h + \frac{\lambda_\alpha}{2}(\nabla_\alpha h)^2 - K\nabla^2(\nabla^2 h).$$

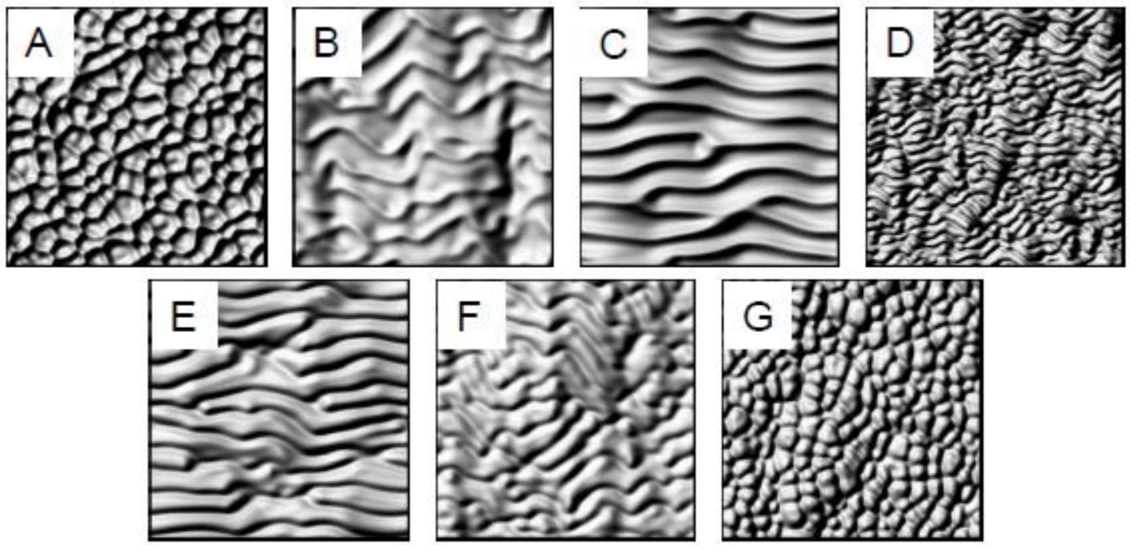


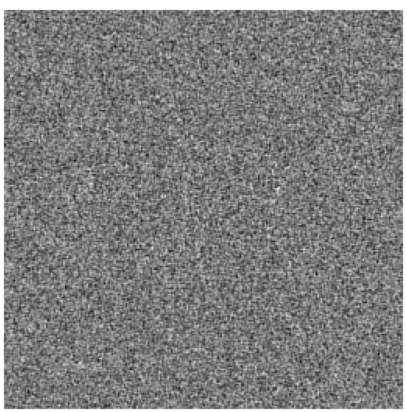


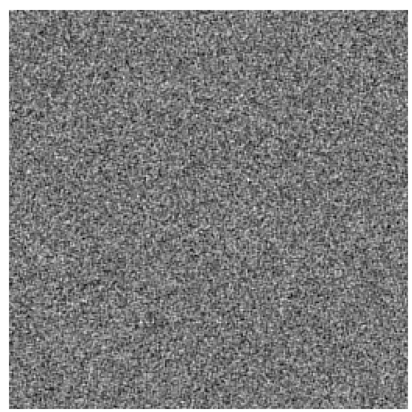


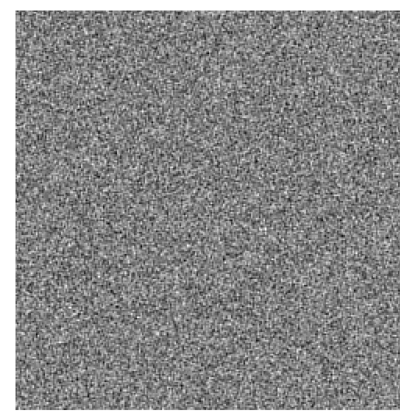
Еволюція поверхні при розпорошенні

$$\partial_t h = \gamma \nabla_x h + \nu_\alpha \nabla^2_{\alpha\alpha} h + \frac{\lambda_\alpha}{2} (\nabla_\alpha h)^2 - K \nabla^2 (\nabla^2 h).$$









Дякую за увагу