Diffusional dependent structures on the crystal surface

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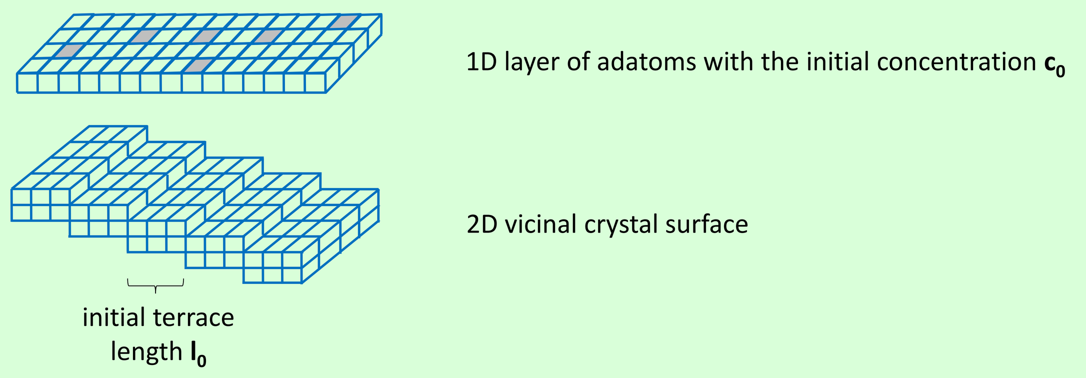
Different patterns can be created on the surface of growing crystals. The Ehrlich–Schwoebel (ES) effect at the surface steps is considered one of the "usual suspects" of such patterning. The combination of a direct and inverse step barrier and the proper selection of the potential of the well between them or changing the height of the direct step barrier leads to the growth of nanocolumns, nanowires, and nanopyramids or meanders, in the same system [1]. Based on our (2 + 1)D vicinal Cellular Automaton model [2,3,4] we show that not only the combination of step barriers is crucial in the formation of surface structures. In particular, we show that changes only in the diffusion process can lead to different patterns.

(2+1)D vicinal Cellular Automaton model

Model consists of **two** different **modules**:
- the **Cellular Automaton** (CA) one responsible for the evolution of the vicinal crystal surface realizing the growth events
- the **Monte Carlo** (MC) one representing a diffusive lattice gas of atoms deposited at the surface which are chosen randomly atom by atom

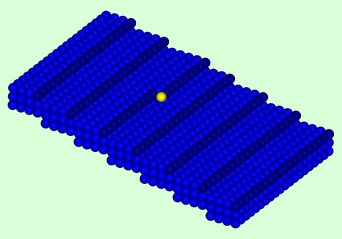
The model consists of two parts:



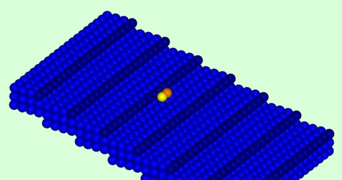
1 time step ($\mathbf{t_{step}}$): → the realization of CA → the MC part → compensation of adatom concentration to its initial value c_0.

Rules:

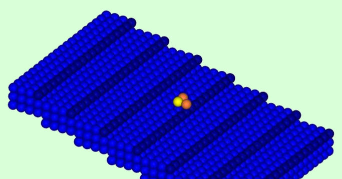
There are 3 different situations when an adatom builds into the crystal:
- when it is at a kink



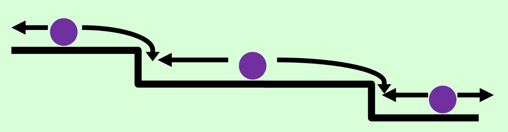
- when a particle adjacent to a straight step and at the same time to another adatom



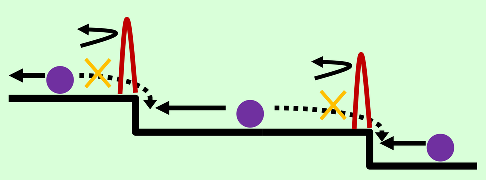
- when the adatom becomes a nucleus for a new layer



Diffusion of adatoms.



In any diffusional update a total number of adatoms is chosen at random, then tried to jump left or right with some probabilities ***P***. Diffusing adatoms make many hops ($\mathbf{n_{ds}}$) before being eventually captured by the growing surface.

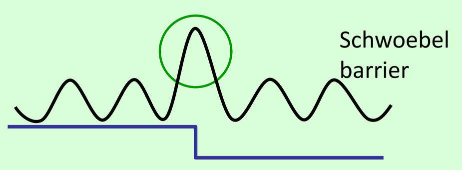


When ES barrier is present in the system the diffusional hops to one direction are inhibited. The source of this barrier is the potential coming from the dangling bonds at the steps which all diffusing atoms feel.

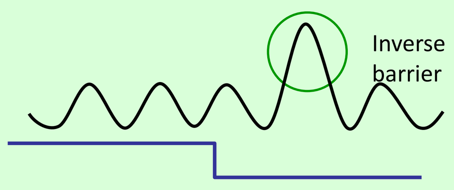
P = 0 – infinite barrier
P = 1 – no barrier

Energy landscape for diffusing particles

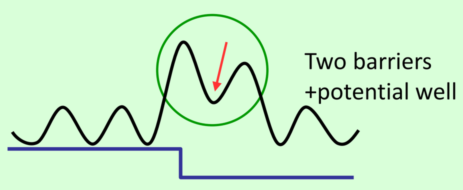
Direct Ehrlich–Schwoebel barrier at the top of the step with jump probability $\boldsymbol{P_{dES}}$



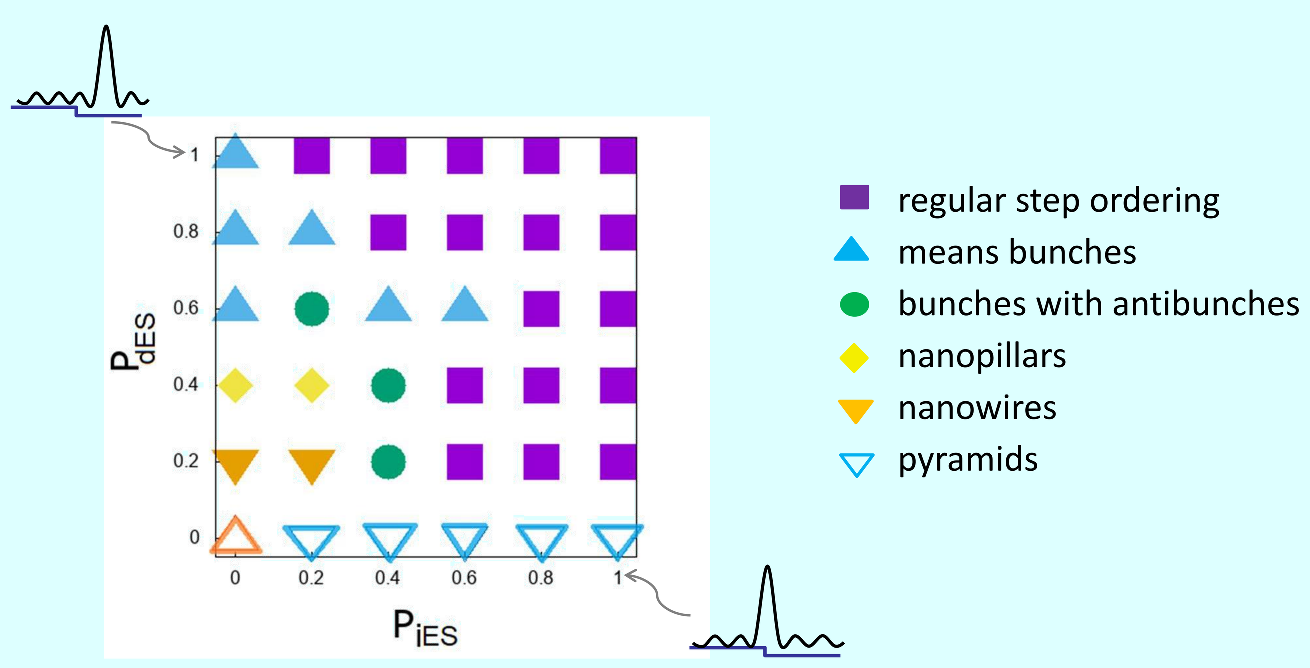
Inverse Ehrlich–Schwoebel barrier in front of the step with jump probability $\boldsymbol{P_{iES}}$



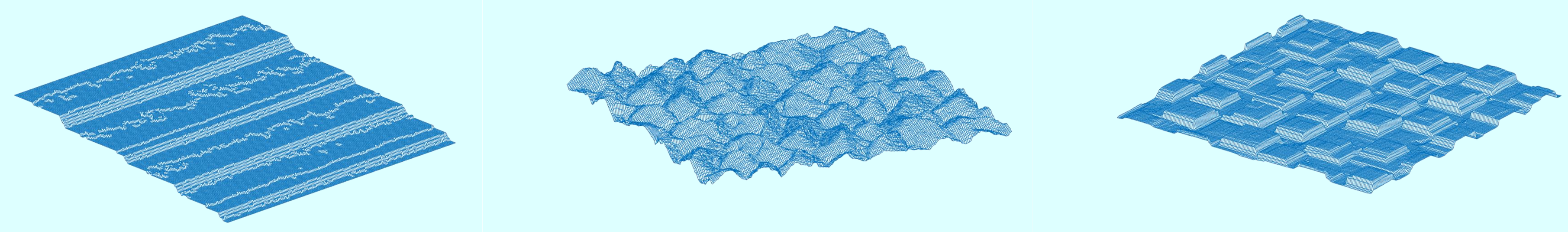
Both barriers and the potential well between them with jump probability out of the well $\boldsymbol{p_W}$



Possible to obtain patterns formation



Examples of possible surface patterns



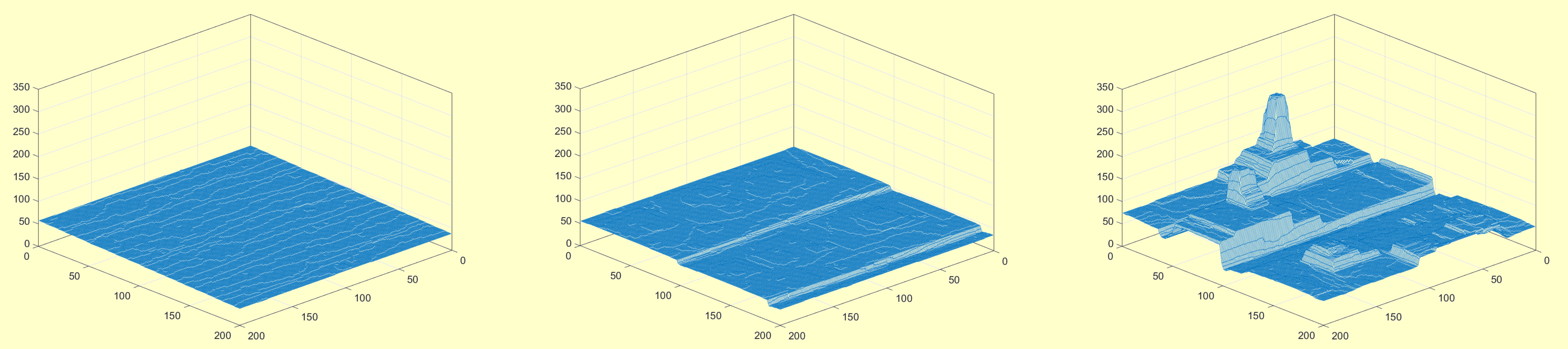
Step bunches *Pyramids* *Nanopillars*

Diffusion rate changes

For all presented results x and y direction are the structure dimensions while z direction is related with the number of particles at particular site. The square or rectangular shape of the structures follows the lattice symmetry.

With increasing n_{ds} is realized a transition from diffusion-like growth to the kinetic-like growth.

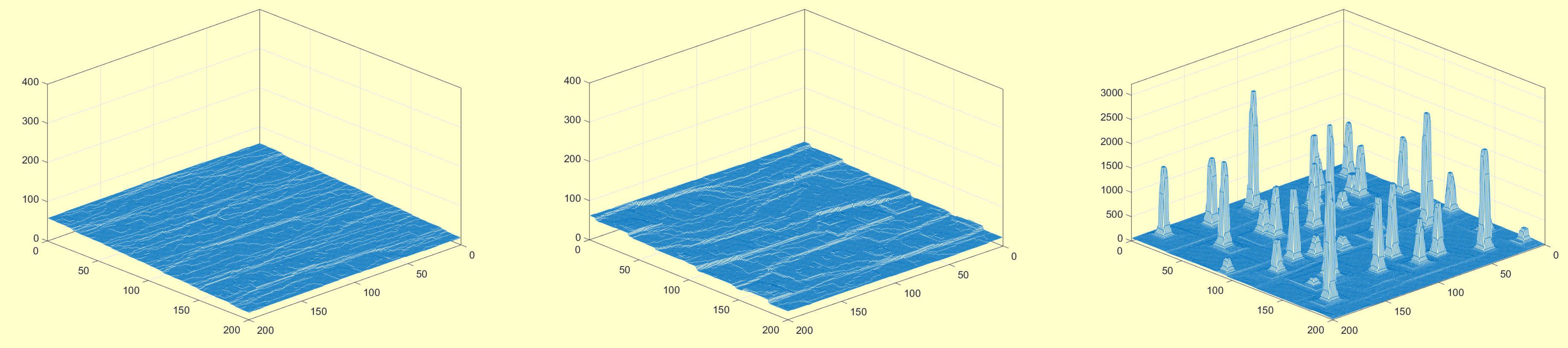
$\boldsymbol{P_{des} = 0.5, P_{ies} = 0.4, p_w = 2.0, c_0 = 0.02, l_0 = 10, t_{step} = 2\times10^5}$



$n_{ds} = 5$ $n_{ds} = 30$ $n_{ds} = 100$

An increase of the diffusion rate leads the final structure from smooth surface trough step bunches to the creation of the nanowires.

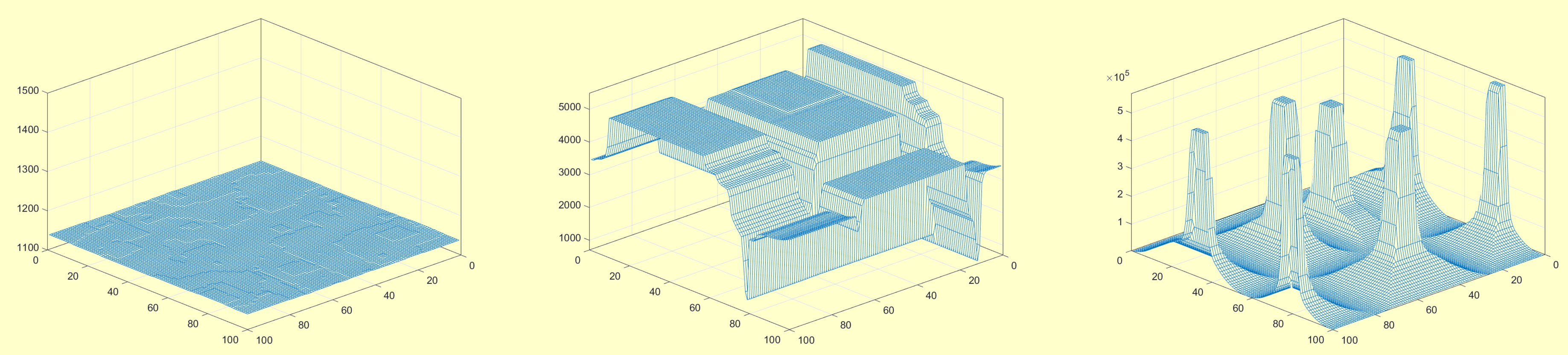
$\boldsymbol{P_{des} = 0.2, P_{ies} = 0.3, p_w = 3.33, c_0 = 0.02, l_0 = 5, t_{step} = 10^5}$



$n_{ds} = 5$ $n_{ds} = 20$ $n_{ds} = 70$

An increase of the diffusion rate leads the final structure from the step bunches to nanowires.

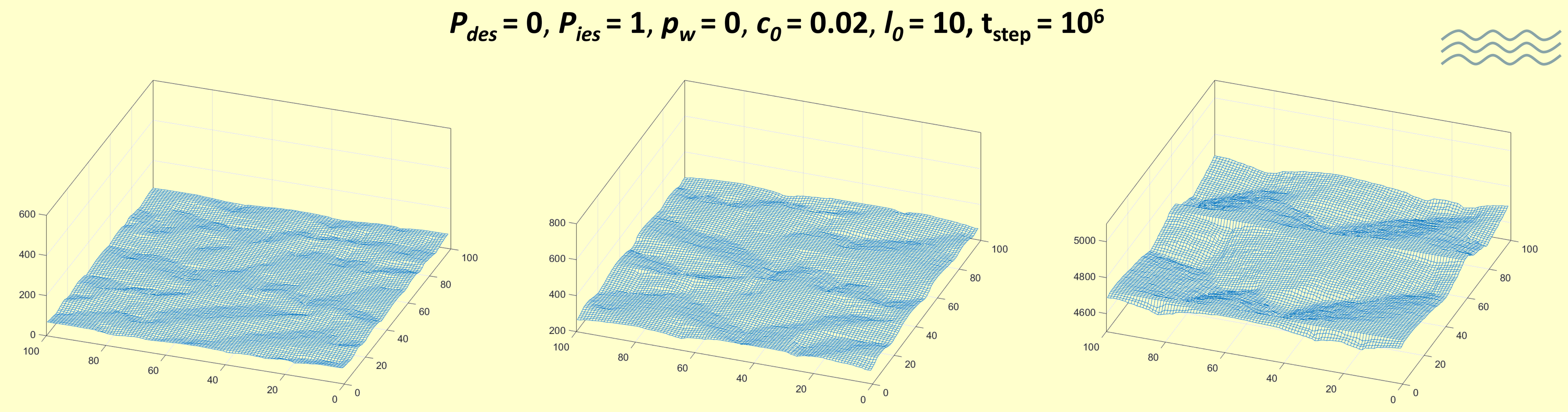
$\boldsymbol{P_{des} = 0.2, P_{ies} = 0.4, p_w = 2.50, c_0 = 0.02, l_0 = 100, t_{step} = 10^7}$



$n_{ds} = 5$ $n_{ds} = 20$ $n_{ds} = 60$

An increase of the diffusion rate leads the final structure from smooth surface trough broad nanopillars with so called cracks to nanocolumns.

$\boldsymbol{P_{des} = 0, P_{ies} = 1, p_w = 0, c_0 = 0.02, l_0 = 10, t_{step} = 10^6}$



$n_{ds} = 1$ $n_{ds} = 10$ $n_{ds} = 60$

An increase of the diffusion rate leads to a longer meanders wavelength

Conclusions

Using (2+1) vicinal Cellular Automaton model we obtained different surface structures.

We observed that it is possible to obtain different surface structures only by changing the diffusion process.

References:
[1] M. Załuska-Kotur, H. Popova and V. Tonchev, ***Crystals*** 11, 1135 (2021).
[2] F. Krzyżewski, M.A. Załuska-Kotur, A. Krasteva, H. Popova and V Tonchev, ***Cryst. Growth Des.*** 19, 821 (2019).
[3] F. Krzyżewski, M.A. Załuska-Kotur, A. Krasteva, H. Popova and V Tonchev, ***J. Cryst. Growth*** 474, 135 (2017).
[4] A. Krasteva, H. Popova, F. Krzyżewski, M. Załuska-Kotur, M. and V Tonchev, ***AIP Conf. Proc.*** 1722, 220014 (2016).