Modeling and characterization of surface patterns formed on the surface of a growing crystal

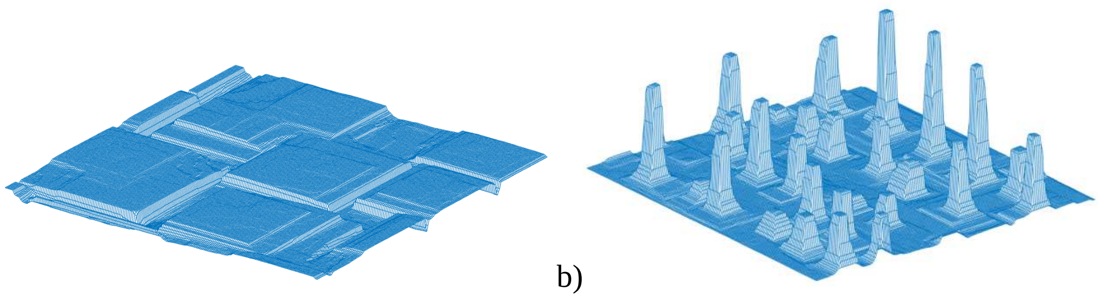
M. Chabowska[1], H. Popova[2], V. Tonchev[3], M. Załuska-Kotur[1]

[1]*Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, PL-02668 Warsaw, Poland*
[2]*Institute of Physical Chemistry, Bulgarian Academy of Sciences "Acad. G.Bonchev" str., 1113 Sofia, Bulgaria*
[3]*Faculty of Physics, Sofia University, Sofia, Bulgaria*

E-mail: galicka@ifpan.edu.pl

Formation of various geometric patterns on the surface during crystal growth process remains a subject of interest of many researchers. Step-bunches, meanders, nanowires, islands, mounds of different shapes are structures that are usually sought as a basis for implementing new solutions at the nanoscale. An important mainspring behind such searches is the use of nanostructures as a solid platform for topologically protected quantum computing. An identification of growth conditions to obtain such structures is important to maintain proper control under the nanostructures production process Therefore, good theoretical surface modeling is essential to create well-defined and structured crystalline substrates that are ready to be used in research and technological processes.

It is the particle diffusion in the presence of step-edge barrier that drives the surface of the growing crystal towards a well-defined ordering. The diffusion of particles in the inhomogeneous potential energy landscape leads to many unexpected and interesting behaviors of the system. The combination of the direct and inverse step barrier and the proper selection of the well potential between them or the change in the height of the 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 [3,4] we analyze the above-mentioned different structures on the crystal surface (Fig.1). Therefore we investigate the surface characteristic through analysis of the two length scales: height and horizontal distance. We show that proper identification of length scaling allows for pattern identification in a simple, automatic way. As an effect we are able to analyze surface stability diagrams for different model parameters in the context of surfaces obtained experimentally for grown GaN crystals.



a) b)

Fig. 1. Structures obtained for initial concentration of particles c_0=0.02, a) inverse Ehrlich-Schwoebel barrier with jump probability given by P_{ies}=0.1, direct Ehrlich-Schwoebel barrier with jump probability given by P_{des}=0.44, the energy of particle that stays at the bottom of the step p_w=2.22, length of terrace l_0=10 and number of diffusional steps n_{DS}=10 which leads to nanopillars b) P_{ies}=0.2, P_{des}=0.4, p_w=2.5, l_0=2, n_{DS}=40 which leads to nanowires. System size 200 x 200.

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