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”Devil’s staircase” of phase transitions in the model of dimer adsorption: computational study of thermal stability

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The term “devil’s staircase” of phase transitions is used to refer to an infinite sequence of ordered phases in a finite volume of the phase space. This phenomenon has a great potential for production of two-dimensional nanoscale objects, because one can create an infinite number of different ordered structures with different cell periods and properties using only one type of building blocks (molecules in particular case) [1]. Understanding of the patterns and driving forces of self-organization in such systems can be employed for production of nanoelectronic devices (molecular electronics, sensors, functional surfaces, etc.) and of highly-selective heterogeneous catalysts.
Recently we have proposed the adsorption model for dimer molecules on hexagonal lattices [2] and have discovered the “devil’s staircase” phenomenon for the ground state of the model. In this case the key factor causing the emergence of an infinite number of ordered structures in a finite phase space volume is the presence of two concurrent types of adsorption –horizontal and vertical adsorption of dimer. Lateral interactions between adsorbing species are simple and short-range –hard-wall potentials, which prohibit adsorption on nears-neighbor sites of already adsorbed molecules.
The existence of the “devil’s staircase” for the ground state of the model do not guarantee its existence for non-zero temperature.
In this work we have confirmed that the sequence of ordered phases of dimers on hexagonal lattice persists at non-zero temperatures. It was shown that least five ordered phases are stable through two numerical methods in the SUSMOST code [3]: transfer-matrix and Monte Carlo (Fig.1).

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[1] Y. Ye, W. Sun, Y. Wang, X. Shao, X. Xu, F. Cheng, J. Li, and K. Wu, The Journal of Physical Chemistry C 111, 10138 (2007).
[2] V. Fefelov, V. Gorbunov, A. Myshlyavtsev, M. Myshlyavtseva, and S. Akimenko, Adsorption 19, 495 (2013).
[3] http://susmost.com/

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