Nanostructured surfaces

Monte-Carlo simulation of non-equilibrium self-organization of nanoparticles on a substrate

N.I. Lebovka

[1] *Institute of Biocolloidal Chemistry, NAS of Ukraine, 42 Vernadsky Prosp., Kyiv-03142, Ukraine*

The random sequential adsorption (RSA) is frequently used for simulation of self-organization of nano-particles on a substrate. RSA assumes that the newly placed particle cannot overlap with the previously deposited ones and the final state is a disordered one (known as the jamming state). The fraction of the total surface occupied by the adsorbed particles is called as the jamming concentration, p_j. The extended particles with different shapes and sizes (e.g., linear and flexible (polymer-like)k-mers (particles occupying k adjacent sites), T-shaped objects and crosses, squares, disks, ellipses [1,2] have been studied and data shown that value of p_j depends strongly on the object shape and size. The percolation in films of extended particles and their mixtures on a substrate was also intensively studied [3]. This approach was shown to be useful for explanation the experimental data on percolation in segregated polymers [4]. The present work reviews the effects of non-equilibrium self-organization for different shapes of extended objects and types of inter-particle correlations. The finite-size scaling, packing, percolation and electrical conductivity behavior in elongated systems (strips) is also discussed. The proposed models are suitable for reasonable explanation of experimental data for different physical systems.

The author acknowledges the partial financial support of project 43-02-14(U), Ukraine.

1. *Evans, J. W.* Random and cooperative sequential adsorption // Rev. Mod. Phys. -1993. -**65**. –P. 1281–1329.
2. *Lebovka, N. I., Karmazina, N. N., Tarasevich, Y. Y., Laptev, Y. Y.* Random sequential adsorption of partially oriented linear k-mers on a square lattice // Phys. Rev. E -2011. -**84**. -P 29902.
3. *Tarasevich, Y.Y., Lebovka, N.I., Laptev, V. V.* Percolation of linear k-mers on a square lattice: From isotropic through partially ordered to completely aligned states, Phys. Rev. E – 2012. -**86**. –P. 61116.
4. *Lebovka, N., Lisunova, M. , Mamunya, Y. P. , Vygornitskii, N.* Scaling in percolation behaviour in conductive-insulating composites with particles of different size // J. Phys. D. Appl. Phys. -2006. -**39**. –P. 1–8.