## Evolutionary prediction of 2D materials formation on substrates

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Successful synthesis of graphene opens a new possibility of formation of fundamentally new low-dimensional materials: ultrathin films with atomic thickness with unique physical properties. At the first stages 2D films were obtained by mechanical exfoliation from the crystals having layered structure (graphene, h-BN, $MoS_2$[1], etc.), while further two-dimensional materials with structure and properties having no analogues in 3D (as silicene[2], borophene[3], CuO[4], Fe[5], FeO[6], CoC[7] etc.) were synthesized. Important that there is a very limited set of methods for simulation of the formation process of nanostructures and can only partially describe the formation of nanostructures. Necessary conditions for obtaining the desired material during the growth process is the correctness definition of the main parameters: the type and composition of the substrate, the external conditions (temperature and pressure), the definition of the necessary parameters of the cells of the substrate and the desired material, as well as their symmetry. Here we presented an effective method for simulation of formation of two-dimensional materials with one and several layers thickness on substrates of different composition using Evolutionary algorithm USPEX. New expanded modules of the USPEX software allow to simulate the formation of low-dimensional nanostructures and predict the crystal structure of low-dimensional materials with random composition consisting of more than 2 types of atoms on different substrates depending on external parameters (temperature, pressure). Applied extended USPEX modulus simulation of the formation of 2D nanostructures with several layers thickness of a given composition (including NaCl, LiCl) on various substrates (including Cu, Ni, Ag, graphene, diamond) as well as the formation of novel 2D-CuO[3] layer in bilayered graphene nanopore were carried out. Obtained results has an excellent agreement with available experimental data. Authors acknowledge the financial support of the RSF according to the research project No. 18-73-10135.

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