ТЕЗИСЫ ДОКЛАДОВ

INTERNATIONAL WORKSHOP

«Multiscale Biomechanics and Tribology of Inorganic and Organic Systems»

МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ

«Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций»

VIII ВСЕРОССИЙСКАЯ НАУЧНО-ПРАКТИЧЕСКАЯ КОНФЕРЕНЦИЯ С МЕЖДУНАРОДНЫМ УЧАСТИЕМ, ПОСВЯЩЕННАЯ 50-ЛЕТИЮ ОСНОВАНИЯ ИНСТИТУТА ХИМИИ НЕФТИ

«Добыча, подготовка, транспорт нефти и газа»

Томск
Издательский Дом ТГУ
2019

DOI: 10.17223/9785946218412/153

MODELING OF THE DYNAMIC OF SELF-ASSEMBLY BOROPHENE BY PFC

[1]Zapolsky H., [2]Bobenko N., [2]Ponomarev A., [2]Khon Yu.
[1]Rouen university, Rouen, France
[2]Institute of the strength physic and materials science, Tomsk

Self-organization of the structure is one of the most promising ways to develop new materials with high physical properties. The phase field crystal method (PFC) appeared as the most preferred choice for studying these phenomena on mesoscale and can be supplementary to molecular dynamics (MD) and the Monte Carlo method (MC), taking into account the limitations of MD and MC computationally in a very effective way. In last years, the phase field crystal equations have also been improved [1,2], to take into account the effects of atomic scale: a characteristic of a polyatomic system has been introduced in terms of quasiparticles (phratons); A new simple form of phenomenological model potentials describing the direction, length and strength of the atom-atom bond is proposed, and the kinetic equations of the atomic density field theory (ADF) are used, describing diffusion on the atomic scale [3]. In our work, we use PFC to simulate the dynamics of self-assembly of a two-dimensional borophene structure. Borophene (two-dimensional sheet boron) - 2D new type of material which is grown on single crystal substrates in ultrahigh vacuum conditions [4] and, depending on the growth conditions, may have some modifications [5]. In this work, we studied the Pmmn2 modification of borophene, which in the structure of atomic clusters is similar to graphene layers with an additional atom in the center of the hexagon.

To simulate the borophene growth stages by the PFC method, the atomic distribution function was obtained:

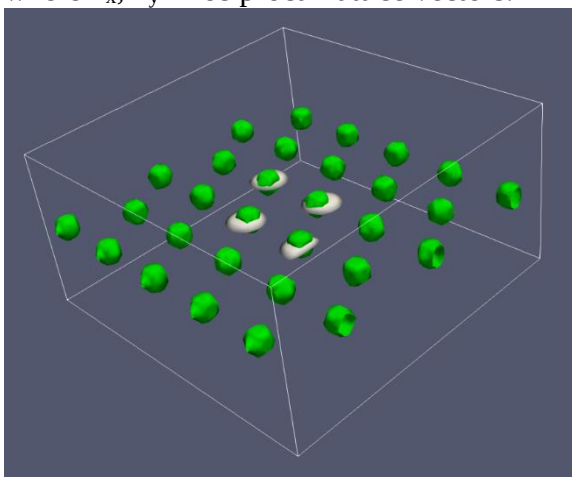
$$f(x,y) = \cos\left(\frac{ax}{2}\right) cos\left(\frac{\sqrt{3}ay}{2}\right),$$

where a – lattice parameter of borophene.

Interatomic interaction potential has the following form:

$$V(k_x, k_y) = 4cos\left(\frac{\pi}{a}k_x\right) cos\left(\frac{\pi}{\sqrt{3}a}k_y\right),$$

where k_x, k_y – reciprocal lattice vectors.



Borophene structure modeled by the PFC. The initial structure is marked in white, the grown borophene 2D sheet is green in green.

In Fig. white color indicates the initial atoms; green — the final structure of borophene, which is obtained by redistributing the density of phratons into one layer with a gradual increase in the density and diameter of boron atoms.

Modeling a borophene 2D structure using the PFC method allows us to mark the growth dynamics of this material.

1. M. Lavrskyi, H. Zapolsky, and A.G. Khachaturyan. Fraton theory and modelling of self- assembling of complex structures // ArXiv: 1411.5587. 2014.
2. M. Lavrskyi, H. Zapolsky, and A.G. Khachaturyan. Quasiparticle approach to diffusional atomic scale self-assembly of complex structures: from disorder to complex crystals and double-helix polymers. // Npj Computational Materials. 2016. № 2. P. 15013.
3. G. Demange, M. Chamaillard, H. Zapolsky, M. Lavrskyi, A. Vaugeois, L. Lunéville, D. Simeone, R. Patte. Generalization of the Fourier-spectral Eyre scheme for the phase-field equations: application to self-assembly dynamics in materials. // Comput. Mater. Sci. 2018. № 144. P. 11-12.
4. Mannix, A.J., Zhou, X.-F., Kiraly, B., Wood, J.D., Alducin, D., Myers, B.D., Liu, X., (...), Guisinger, N.P. Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. // Science. 2015. № 350. P. 1513-1516.
5. Wang, ZQ., Lü, TY., Wang, HQ. et al. Review of borophene and its potential applications. // Front. Phys. 2019. № 14. P. 33403.