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The features of diamond nucleation on nanolevel prediction of diamondization of multilayered graphene

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Since the isolation in 2004 graphene continues to attract significant attention from the scientific community. Despite of the fact that graphene is under detailed investigation more than 10 years it still serve as a source for unusual effects. Here I will show that multilayer graphene surface can be used a base for formation of diamond nanofilms [1] facilitated by chemical adsorption of adatoms on the multilayer graphene surface, and explain how the pressure of phase transition is reduced and formally turns negative. For the first time we obtain, by *ab initio* computations of the Gibbs free energy, a phase diagram (P, T, h) of quasi-two-dimensional carbon—diamond film versus multilayered graphene. It describes accurately the role of film thickness h and shows feasibility of creating novel quasi-2D materials. In such “chemically induced” phase transition both chemistry and compression concurrently serve as the driving factors for diamond film formation. I will continued to discuss this effect through the ultrastiff films with hexagonal diamond (lonsdaleite) type structure and further show that under the particular external conditions and using particular adsorbate atoms films with the specific structure can be formed [3]. The process of diamond phase nucleation was further investigated on the atomic level. The critical size of graphene hydrogenated region which can initiate graphene diamondization was estimated. The nonlinear dependence of size of graphene hydrogenated region upon the number of layers predicted the maximal thickness of the film which can be formed by chemically induced phase transition [3]. This research was supported by Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST «MISiS» (№ K2-2015-033).

1. A.G. Kvashnin et al. Nano Letters 14 (2014) 676
2. L.Yu. Antipina et al. J. Phys. Chem. C 119 (2015) 2828
3. S.V. Erohin et al. submitted (2017)

Biography

Pavel Sorokin has completed his PhD at the age of 25 years from Lebedev Physical Institute of RAS, Moscow and postdoctoral study from Rice University. He is the leading researcher of Inorganic Nanomaterials Laboratory in National University of Science and Technology "MISiS". He has published more than 80 papers in reputed journals.

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