Research of the nanopour creation mechanism at the thin-filmed systems of the different nature

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Recently one of the most perspective direction of the nanoelectronic becomes a creation of ordered arrays of the nanocrystals at the porous of the thin films different nature, which have novel physical properties. It is due to their develop surface and quantum dimensional effect.The most famous materials for preparation thin-filmed systems are graphene films, films of $\gamma - Al_2O_3$ and films of silicon oxide. But there is no theoretical research of these objects till present time.

That's why in our paper we report about calculations of the vacancy creation mechanism at the graphene layer and at the surface of aluminum oxide $\boldsymbol{\gamma} - Al_2O_3$ to prove the possibility of the nanopour creation mechanism in these thin-filmed systems.

As a geometric model of thin film graphene film and film of $\boldsymbol{\gamma} - Al_2O_3$ were used. The research was carried out by applying the Molecular Cluster model (MC) and semi empirical quantum-chemical MNDO scheme. Graphene film cluster consiSt of 60 carbon atoms. As a basic model for $\boldsymbol{\gamma} - Al_2O_3$ layer building crystal lattice of spinel, in which Mg atoms were changed on Al atoms, was used [1].The process of the vacancy creation at the surface of graphene and $\boldsymbol{\gamma} - Al_2O_3$ films has been modeled by step-by-step removal (minimal step 0.1 A) of carbon and aluminum atom from the surface of the film respectively till their full break-off. Geometry of the system was optimized on the each step. The analysis of energy curves of these processes show that there are two extremum on it: minimum and maximum. Minimum of the energy corresponds to stable state of the thin-filmed system. In that state carbon or aluminum atom is located near to the film surface. Maximum of the energy corresponds to activation energy of the vacancy defect. This fact caused the creation of different topological structures near the place where the vacancy located. This defect might be called nanopour.

The theoretical findings were experimentally confirmed by growing the porous aluminum oxide by electrochemical method. Analysis of the oxide surface's topology showed that there are periodically arranged pore diameter of 26 nm in it.

So, we have proved the possibility of nanopour's creating on the surface of filmed systems, which can become a place, where arrays of nanocrystals of different metals can be further formed.

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[1] Litinskij A.O., Gohbere P. Ja, Shatkovskaja D.B., Bolotin A.B., Litinskaja N.N., Popov G.P. *TEC* 19(4) 486 (1983).