

Registration of the process of nanodiamonds formation of various sizes

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Nowadays nanodiamonds is widely used in a lot of different areas and its synthesis is one of the necessary and actual questions. The detonation products of HEs with a negative oxygen balance contain a wide phase and morphological variable of carbon forms. This forms of condensed carbon in detonation products depend on the explosion conditions. So that development of the detonation methods for the synthesis of various forms of nanodiamonds is primarily motivated by their commercial and advanced applications.

This paper presents the experimental results of carbon nanodiamonds synthesis during the detonation of various high explosives (TATB (triaminotrinitrobenzene), composition TNT/RDX (50/50), BTF (benzotrifuroxan) and mixture RDX with graphite).

In this work we used different methods: dynamics registration of small-angle x-ray scattering signal during the detonation, high resolution transmission electron microscopy and x-ray diffraction studies of the recovered carbonaceous residue (soot) of these high explosives.

The results demonstrate the different kinetics of carbon condensation process during the detonation of HEs and different sizes of nanodiamonds (from nanometers to microns).

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Properties of "boron+vacancy" complexes in diamond surface layers

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Synthetic diamond single crystals are currently an active area of research. The combination of unique properties makes diamond a promising material for many high-technology fields. The most important surfaces of a CVD diamond are the C(100) and C(111) surfaces. It is known that the *p*-type conductivity arises from doping diamond with a boron impurity. In this paper, we present the results of quantum-chemical modeling of the configurations of boron impurities, as well as "boron+monovacancy" BV-complexes, varying their positions in the C(100)-(2×1) and C(111)-(2×1) near-surface layers of diamond. Calculations of the geometric, electronic, and energy characteristics of diamond clusters C₁₉₅H₁₁₂B and C₁₂₂H₇₉B simulating a clean reconstructed surface and containing a boron atom as a substitutional impurity, were performed by the *ab initio* method of Hartree-Fock (a Firefly QC software package [1]), and using semi-empirical quantum chemical methods implemented in the MOPAC software package [2]. It has been found that the most stable positions of boron on the C(100)-(2×1) diamond surface are the configurations in which the B atom replaces one of the dimer atoms, or is in the third layer under the dimer row. A stable "boron+monovacancy" BV-complex is a state where the boron atom replaces the fourth-layer C atom, and the vacancy is in the third layer under the dimer rows, while a hexagonal "graphene-like" structure of atoms bound by π -conjugation is formed on the surface. A stable configuration on the C(111)-(2×1) diamond surface is the one where the B atoms replace the carbon atoms of the Pandey chains. The stable state of the BV-complexes in the chains has been determined.

This study illustrates that the impurity boron atoms and BV-complexes in the near-surface layers of diamond lead to a significant change in the geometry and electronic state of the surface affecting its adsorption and vibrational properties.

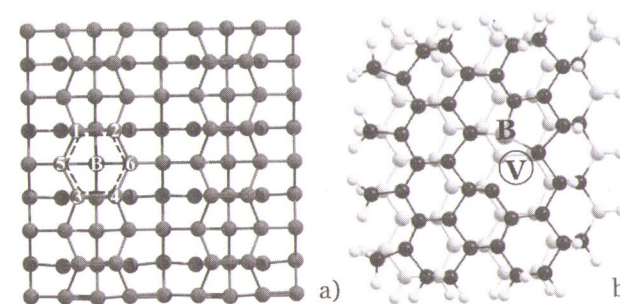


Fig.1. Fragments of diamond clusters, top view: a C(100)-(2×1) surface, boron in the third layer (a); a C(111)-(2×1) surface, boron in the first layer, top view (b).

References

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