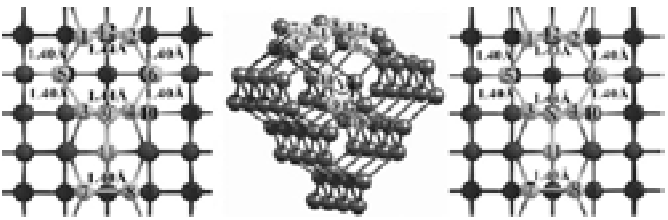
Adsorption properties of the diamond C(100)-(2×1) surface containing vacancies and nitrogen - vacancy defects

Natalia Lvova
Natalia Lvova and Anna Ryazanova, MIPT, TISNCM, Russia

The nitrogen - vacancy complexes (NV complexes) determine the useful properties of nanodiamond fluorescence [1]. Single nitrogen - vacancy defects in diamond consist of a carbon-substituting nitrogen atom (N) and a vacancy (V) located in the neighboring lattice point [2]. In order to use the NV center, it should be located in a nanometer-size diamond particle. In our recent paper [3], we found that the most stable position of the vacancy in the near-surface layers of the clean surface C(100)-(2×1) is the defect position in the third layer directly under the dimer row of the upper layer, and for the complex defect nitrogen - vacancy is configuration «vacancy in the third layer, nitrogen in the fourth layer» [4]. In this study, the energy characteristics of hydrogen chemisorption on the C(100)-(2×1) diamond surface with vacancy defects and nitrogen - vacancy complexes in singlet and triplet states are investigated using quantum chemistry methods using semi-empirical quantum chemical methods on the C195H112 cluster. Modeling of the hydrogenated surface is traditionally used to determine the overall passivation effect [5]. The main conclusion of this study was shown that the most active centers for hydrogen adsorption are atoms of the surface hexagon, formed from the atoms of the upper and the second layers when a vacancy occurs in a third layer. However, the specific values of the energy characteristics depend on the nature and state of the defect.



Recent Publications

1. Tsukanov A.V. (2012) NV-centers in diamond. Part I. General information, fabrication technology, and the structure of the spectrum. Russ. Microelectr.41:91.
2. Jelezko F., Wrachtrup J. (2006) Single defect centres in diamond: A review. Phys. Stat. Sol.(a) 203:3207
3. Lvova N.A., Ponomarev O.V., Ryazanova A.I. (2017) Vacancies in the C(100)-(2x1) diamond surface layers. Comput. Mater. Sci. 131:301.
4. Ponomarev O.V., Ryazanova A.I., Lvova N.A. (2018) Nitrogen-vacancy defects near the C(100)-(2×1) diamond surface. Surf. Sci. 667:92
5. Bradac C., Gaebel T., Naidoo N. et al. (2009) Prediction and measurement of the size-dependent stability of fluorescence in diamond over the entire nanoscale. Nano Lett. 9:3555.

Biography

Anna Ryazanova has graduated MIPT in 2018 and has defended her master's degree on theoretical study of point defects in diamond. Currently, she continues her study as a PhD student.

ryazanova@phystech.edu