Structure and characteristics of pyrolyzed polyacrylonitrile with vacancies

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The discovery of new forms of carbon has stimulated interest in the synthesis of new nanomaterials with modified chemical properties that contain carbon plane. These include nanomaterials on the basis of containing carbon pyrolyzed polyacrylonitrile (PPAN). PPAN used in microelectronics, vacuum electronics, optoelectronics. Advantages of the new organic semiconductor based PPAN are regulation of the conductivity, low coSt. and simple technology of preparation [1].

One of the interesting problems is to study the properties of PPAN with vacancies (the so-called V defect). These defects change the local geometry of the layer (see Fig.) and, consequently, the electronic states. Surface of a material with vacancies, as a rule, consists of carbon hexagons and penta- and emerging heptagons (topological defects), which may lead to deformation of the polymer surface. We investigated the electronic structure PPAN with vacancies. Main energy characteristics of processes were calculated. Calculations were performed using quantum-chemical methods MNDO and PM3 and method DFT. Considered two types of defects: 1) V_N defect when removed from the structure of the nitrogen atom, and 2) V_C defect when removed from the structure of the carbon atom. Energy curves illustrating the formation of a vacancy, were constructed. The comparing the characteristics of defect and defect-free structures PPAN was performed. It should be noted an increase in the value of energy the highest occupied molecular orbital E_{HOMO} in the presence of the defect and a corresponding increase in the band gap. Thus, the introduction of a vacancy in the layer structure allows you to modify the physical properties of the material. The geometrical analysis shows that the surface atoms are displaced from their permanent positions in the direction of localization of vacancies. The electron density is localized in the V defect, which in turn leads to a change in the polarization of the monolayer PPAN and change its physical properties.

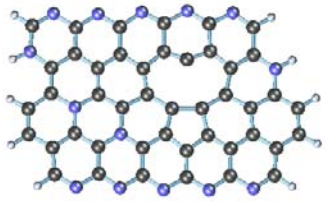

Figure. Monolayer PPAN with defects after optimization of parameters.

[1] V.V. Kozlov, L.V. Kozhitov, V.V. Krapuhin, I.V. Zaporotskova, O.A. Davletova, D.G. Muratov, *Materials of Eelectronic Engineering* № 1, 59 (2008).