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Short Communication

Research of the Vacancy Migration Process on the Surface of BC Nanolayer

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The ionic conductivity and structure in which it cans be realized research is very important for the development of modern batteries. Using of new materials will enable from such deficiencies as little time of life, small energy, and possibility of leak from battery. In this paper we present the results of investigation of ionic conductivity process of boron carbon nanolayers. The research was performed using the MNDO method within the framework of a molecular cluster model and DFT method using B3LYP functional and 6-31G basis. For investigation of ionic conductivity processes the vacancy formation on the nanolayer have been modeled. Energetic and electronic characteristics of these processes have been carried out. The vacancy migration process has been modeled. The conductivity coefficient dependence of temperature has been found.

Keywords: Boron-carbon nanolayers, Vacancy migration process, Ionic conductivity.

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1. INTRODUCTION

Liquid conductors commonly used in batteries and accumulators possess obvious drawbacks, namely short cycle life, low energy capacity and besides they are prone to leakage and spillage [1]. Structures with ionic conductivity can substantially extend cycle life of batteries since they can function both as electrolytes and electrodes simultaneously.

However, one of the main challenges we face when implementing the ionic conduction mechanism is that the size of an ion is often comparable to a distance between the sites of the crystal lattice, which explains why transport of charged ions similar to that one in metals almost never occurs in crystal structures. Therefore, to design a class of solid-state structures with ionic conductivity we need new materials with conduction properties that can be modified by using different methods. Recent studies have found that carbon nanotubes (CNTs) and boron-carbon nanotubes (BCNTs), whose properties and conductive characteristics can be designed by applying different modification methods, can be successfully used as a material for ionic conduction. In [2, 3] the results of research into the mechanism of ionic conductivity in single-walled CNTs and single-walled BCNTs with cylindrical symmetry are presented.

However, nanotubular form can not be regarded as the only way of forming nanostructured materials. Papers [3-7] theoretically predict and describe formation of boron carbide nanostructures. The authors conclude that the calculated 1 : 3 ratio of boron and carbon in them is a clear sign that BC_n type tubular structures, where $n = 3$ are formed. This finding seems to be promising for research into electron and energy characteristics of boron carbon BC_3 tubules as well as ionic conductivity in them similar to that one displayed by carbon nanotubes. But the another form of nanostructured materials may be the quasiplanar layers. This paper presents the results of computer simulation of ionic conductivity in three variants of BC_3 nanolayers with different orientation of boron in them by applying the MNDO method [8] within the framework of molecular and ionic-embedded covalent-cyclic cluster models.

2. VACANCY TRANSPORT PROPERTIES

We investigated energy characteristics of defect migration on the surface of boron-carbon nanolayers. We considered two types of movement for three chemically bonds between neighbouring atoms that we denoted as I and II: I – The vacancy located on the place of boron atom and moves to the carbon atom, II – The vacancy located on the place of carbon atom and moves to the boron atom. They are not equivalent because of the atom orientation features that are discussed in details in [9]. Vacancy transfer along the above described chemical bonds was modeled by using incremental approach of a neighboring carbon (or boron) atom along the virtual C-V or B-V bond to the site of vacancy location. Thus, the surface atom of the nanolayer had two degrees of freedom, which allowed it to move within the surface and freely deviate from it. The geometrical parameters of the other two B and C atoms nearest to the vacancy were fully optimized during the calculation. Therefore, it seemed that the vacancy moved in a direction reverse to the atom migration.

Incremental method allowed us to build energy curves for vacancy transfer process and calculate activation energies (E_a) of the process. The curves (Fig. 1) are qualitatively similar: they have potentional barrier which is located in the middle of the chemical bond. The calculations of the migration processes show that there is one way of vacancy migration for each type of the nanolayer. These ways are: the second variant for A and B type, the third variant for type C. The energy

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barriers have heights of 5.5 eV, and 9.2 eV for these variants, respectively. We identify the barrier with activation energy of the defect. This means that the mechanism of ionic conductivity in the BC_3 nanolayers is energetically favorable, so these nanolayers with predicted conductivity might find application in nanoelectronics.

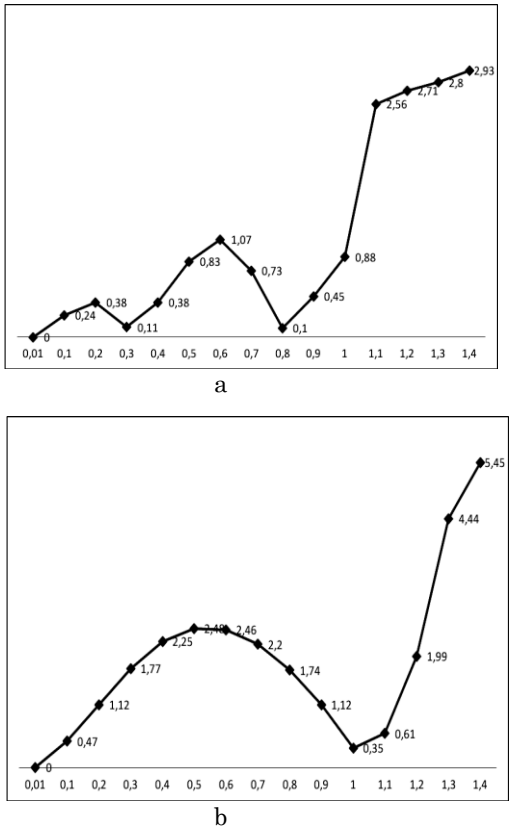

Fig. 1 – The energy curves for defect transfer (vacancy transfer) in BC nanolayers: a) Type A; b) Type B

3. IONIC CONDUCTIVITY IN NANOLAYERS

The analysis of the electronic state of the boron-carbon planar systems with vacancies showed that local electron density redistribution takes place, and atoms closest to the vacancy become charged. Taking it into account, defect migration can actually be thought of as the movement of an ion. Therefore, the calculated activation energies allowed us to investigate dependence of ionic conductivity (the so-called ion hopping conductivity) on temperature according to the well-known formula [10]:

$$\sigma = \sigma_0 \exp\left(-\frac{E_a}{kT}\right), \qquad (2)$$

where k – Boltzmann constant, T – temperature. It should be noted that this formula is valid for low temperatures $kT << E_a$, when we can neglect the temperature dependence of E_a.

The curve revealed a quite significant difference in the conductivity behavior for the three different variants of vacancy transport in three types of boron-carbon nanolayer. Analysis of the migration geometry showed that for migration path II for types A and B formation of topological defect in the shape of a pentagon is observed. While one ion is moving to the vacancy site, the other two can form a chemical bond. The restructuring of the surface change the atomic interactions, which, in its turn, causes changes in activation energies and conductivity of the nanolayer. Pentagons deform the surface, and the layer is distorted. A similar situation was observed in carbon nanotubes[2], when the experimental data showed that deformation of carbon nanotubes surface caused significant (namely, 1.5-fold) changes in their conductivity [11].

4. CONCLUSIONS

We found that introduction of V-defects (vacancy) in the boron-carbon nanolayer causes an increase in the band gap of the defective nanoplanar structures. It means that physical properties of materials can be purposefully changed by introducing defects. Defect migration follows the ways along different bonds and actually represents the process of carbon or boron ions hopping between their stable states on the nanolayer surface. The calculated activation energies revealed that ionic conductivity in boron-carbon nanolayers depends on temperature.

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