BISTABLE STATES OF DEFECTS IN GRAPHENE

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1. Introduction. Graphene is one of the most promising materials in nanotechnology. The electronic and mechanical properties of graphene samples with high perfection of the atomic lattice are outstanding, but structural defects may change their properties /1/. However, deviations from perfection can be useful in some applications, as they make it possible to glue the local fragments of graphene and to achieve new quality. In the article /2/ particular emphasis is put on the unique ability of graphene to reconstruct its lattice around intrinsic defects, leading to interesting effects and potential applications. Defects in graphene were experimentally found /3/ and an increase in density of π-electron states in the vicinity of such defects was mentioned in /4/. It was previously shown (see, e.g., /5/) that in the graphene sheet the 5-7 defect being the convexity of the carbon hexagonal lattice leads to the redistribution of π-electron charges and to the appearance of the local electric dipole moment.

In this work point defects in graphene are considered in the wider frameworks of the carbon surfaces theory. We use the block-regular method, developed by the authors /6/. Graphene consists of a hexagonal monolayer network of sp^2-hybridized carbon atoms. Defects can also be deliberately introduced into graphene, for example, by irradiation or chemical treatments or by making two-dimensional crystals on special surfaces.

2. Description of a fragment boundary. The fragment of carbon surface is limited by a broken line from C C bonds. Usually lines of zigzag or armchair type are considered. Such line can be described (i.e. coded) by binary number (after a choice of orientation of a surface) and by using these binary codes it is easily possible to determine, which fragments can be glued together.

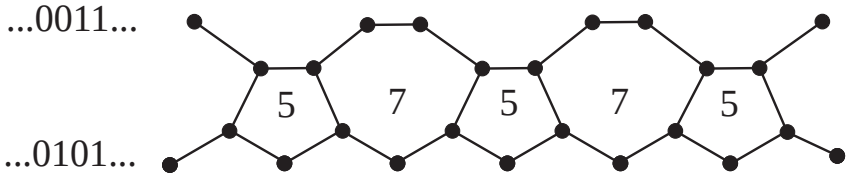


Fig. 1. By using a tape of alternating 5 and 7-gons it is possible to change a zigzag boundary to an armchair one, i.e. from a line with a code $(01)^n$ go to a line with a code $(0011)^k$. So in the defects described by a family of lines-levels 5- and 7-gons are used to change a code of level lines.

A defect can be described as a sequence of such lines. Between nearest lines the tape of polygons is inserted. Some specifications are necessary for

computer processing of such objects. So, between lines it is necessary to insert the closed tape from consistently stuck together polygons (usually 5-, 6- and 7-gons). The polygon is inserted between the next zero of the top line and the nearest unit of the bottom line.

The binary code $b = b_1 b_2 \ \ b_n$ of a line depends on a choice of the start point of the line. The number of zeros of the top line is equal to the number of units of the bottom line and is equal to the number of polygons in a glued tape (see Fig. 1).

Triangles with the sides of length 2 (number of edges) are simple hexagons. Parallelograms have two acute angles (on 60°) and two obtuse angle (on 120°). At blunt corners the wedge is not defined unequivocally. This ambiguity disappears, if for points of graphene layer the hexagons are taken. The triangles are the elementary fragments, but it is possible to add also to them straight lines of type armchair and in general any broken lines given by their binary codes (Fig. 2).

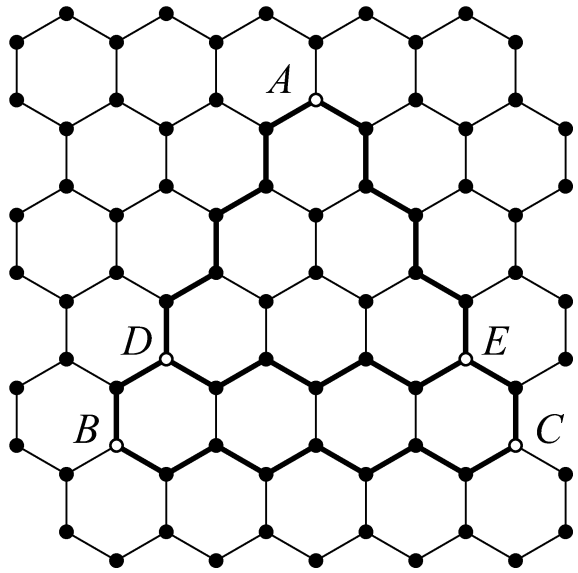


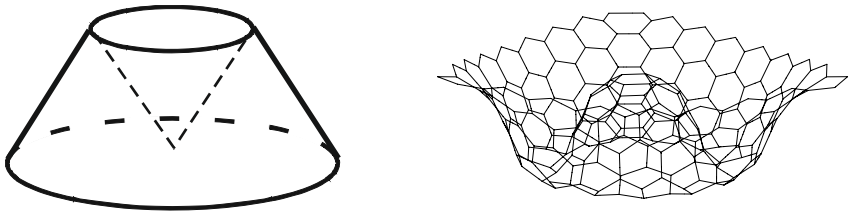
Fig. 2. Equilateral triangle *ABC* with the side length 8 (or 6 hexahons). The triangle *ADE* with the side length 6 is shown too. It is clear, that the side length of such triangles is expressed by even number.

The next step is to determine an arrangement of graphene plane carbon atoms in the vicinity of a given (for example, sequence of binary codes) defects. For this purpose the block-regular method which allows to do it for any carbon surfaces was used. The block-regular structure is given by the set of points and the set of blocks. It is necessary then to arrange these points in the Euclidean space so that the sum of energy of all blocks became minimal. It is similar to the discrete version of a problem to find the minimal smooth surfaces where the area of a surface should take the minimal value.

3. Metastable states. In the work /7/ the form of a surface of a fluid taking into account the electric charges (in external electric field) is discussed in detail. Certainly, because of fluidity its surface is very mobile and consequently is deformed by influence of small forces. Difficulty of a problem is that the deformation of a surface leads to distribution of a charge and, hence, to change of the forces which have caused this deformation.

Carbon surfaces are much more rigid. And still, charges on them can essentially influence on transitions between metastable states (configurations). Two ways of occurrence of set of metastable conditions are shown in Fig. 3. The

ellipse of singular points creates very rigid design. Calculations show, that carbon cones can have similar states.



(a) (b)

Fig. 3. (a) Smooth analogues of metastable states of a carbon cone.
(b) One of metastable states of a carbon cone (with a pressed top).

A metastable state of a cone (almost smooth surface with zero curvature of the interior geometry) is defined by an ellipse made of singular points. If the cone is cut and glued from paper, then transitions between these metastable states are impossible. In Fig. 3a to the singular top the ellipse was added. The region from the points close to top is pressed inside of a cone. Practically for any ellipse (and even for several ellipses) on a cone the corresponding pressed cone exists. These pressed continuous cones have discrete analogues, pressed carbon cones, see Fig. 3b.

4. 5-7 defects in graphene. In this section it is shown, how in a block-regular method the elementary defects are described. After a choice of codes of sequence of level lines, our computer program (written in Mathematica environment) maps points of structure to Euclidean space and by moving them minimizes block energy.

The Stone Wales defect SW(55-77) is formed by rotating a C C bond by 90°. And it leads to reorganization of four C C bonds. For appearance of SW-defect more than 5 eV required accompanied with tunneling through a barrier of $\approx$ 5 eV, see /2/. Formation of several such defects requires not only more energy, it need also a correct choice of reconstructed connections.

Let s consider the defect contained within a triangle with sides made of hexagons (length 5, 5 and 6). Inside of this defect 5- and a 7-gons are located. It is seen in Fig. 4a, that this triangle cannot be inserted into graphene plane. But it is possible to insert into graphene plane two such defects glued into parallelogram which (topologically) has correct border. It is also possible to glue such parallelograms together, which results to unlimited number of carbon surfaces with as much as greater number of metastable states. Two pentagons may be stuck out from a plane in the same or in the different sides. This gives exactly three metastable states. In Fig. 4 one of three possible metastable states of the parallelogram is shown. At realization of this structure (fragment-parallelogram) symmetry (rotations and reflections) is totally or partially broken.

See other defect structures on graphene in /8/.

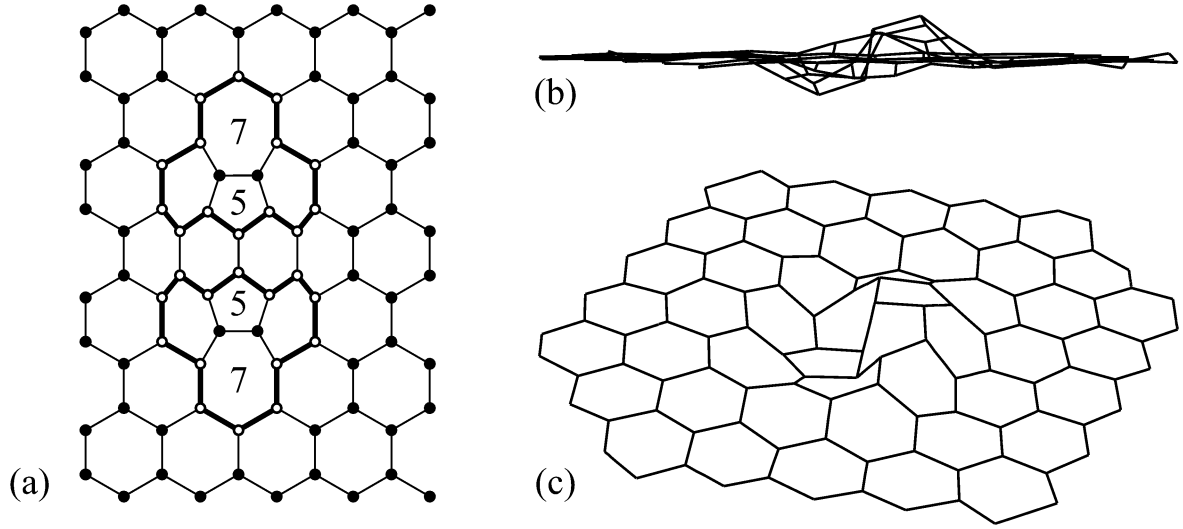


Fig. 4. (a) The structure inside of a regular triangle contains defect and consequently the triangle becomes not regular: two sides of length 4 and one 6. (b) Side view of the defect. It is well visible, that outside of the defect carbon atoms remain in a graphene plane. (c) Top view, hexagons in the vicinity of the defect are strongly deformed.

5. Conclusions. Our calculations show that some defects in graphene may have different metastable states.

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