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COMPUTER GENERATION OF THE MODELS OF LOCALIZED DEFECTS OF CARBON NANOTUBES AND GRAPHENE

Tatiana Grigorenko*, Viatcheslav Barkaline

Belarusian National Technical University, Minsk, Belarus

*e-mail: grigorenochka@mail.ru

Abstract. The research of formation principles of topological defects in graphene layers and carbon nanotubes was carried out in atomistic model approach. The models of defective graphene structures were developed and optimized with molecular mechanics algorithms.

1. Introduction

Graphene layers are the basis of laced carbon nanostructures. The graphene layers consist of carbons in sp2 - hybridization state each and are connected to three adjacent atoms with stable covalent bonds. As a result the atoms are located at the tops of regular hexagons. The formation of carbon nanostructures from graphene layer fragments is the result of topological defect insertion into these layers, i.e. layer reconstruction so that besides hexagons tetra-, penta-, hepta- and octagons are formed in its structure [1].

2. Defective carbon nanostructures

The research of graphene layered structures containing different topological defects was carried out with the help of molecular mechanics methods using MM+ force field.

The structure of graphene layers containing topological defects was analyzed as a part of the research. It was found that topological defects of graphene layers can be divided into simple and complex ones. Simple defects are certain n-gons (n = 3, 4, 5, 7, 8, …) in graphene layer. Complex defects comprise two and more simple defects [1].

Simple topological defects in graphene layer lead to its 3D deformation which entirely deforms the surface. Graphene sheet is bent in different ways depending on the defects sign. The insertion of positive defects 3, 4 and 5 into the layer leads to its bowl-like bent (Fig. 1a). Negative simple defects (7, 8, 9 etc.) leads to saddle-like deformation of graphene sheet (Fig. 1b).

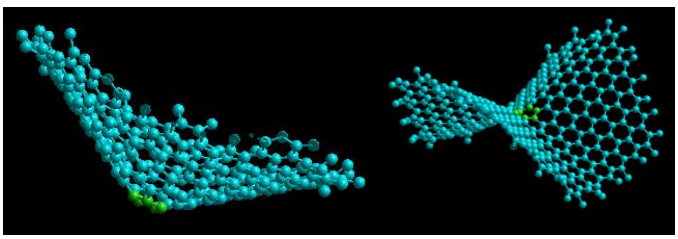


Fig. 1. Graphene layer fragment containing simple topological defect
a) pentagon; b) heptagon.

All complex defects deforming the structure of the layer locally can be divided into two types: point and line defects. 5-7-7-5 and 5-8-5 defects (Figs. 2 and 3) are the examples of point

defects. They may be formed in defect-free graphene sheet by removing several atoms of the layer and reorganizing interatomic bonds.

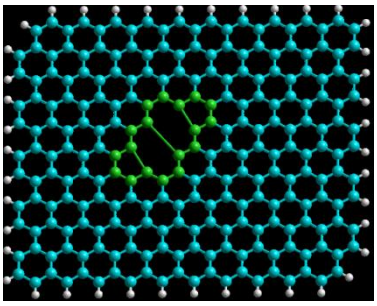


Fig. 2. 5-7-7-5 spot defect.

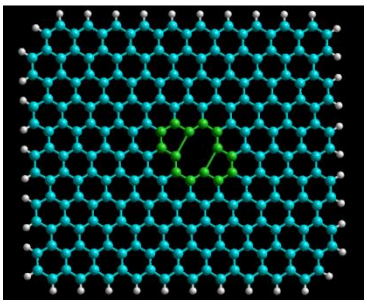


Fig. 3. 5-8-5 spot defect.

5-7-7-5 spot defect can be inserted into the layer using the mechanism depicted in Fig. 4. For instance, for the formation of spot effect it is necessary to remove four atoms from the layer (Figs. 4a and 4b) and then interconnect atoms which have broken bonds (Fig. 4c).

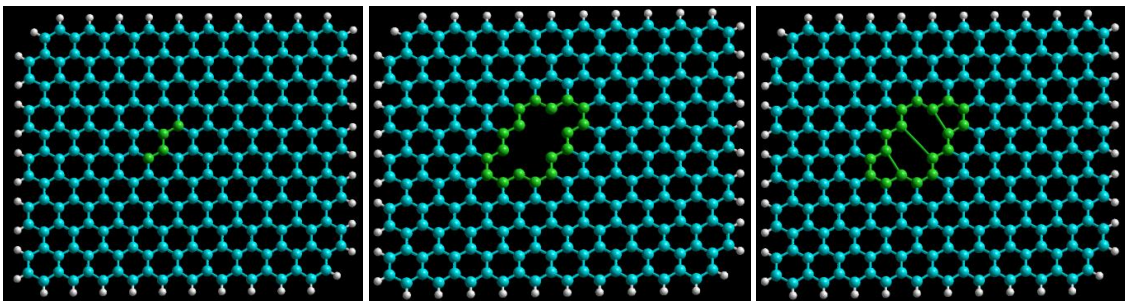


Fig. 4. a) Four atoms in graphene layer to be removed; b) Graphene layer after the removal of four atoms; c) Complex 5-7-7-5 spot defect formed in graphene layer.

The specific feature of spot defects is that they cause the deformation of only small area of graphene layer around the defect.

The second type of defects is line defects. They cause the deformation of graphene layer along a line. Complex 5-7 defect is the example of such defect type (Fig. 5). During modelling line defect can be inserted if the layer is cut from edge to insertion point. After the defect is inserted the layer should be seamed back in the area of cut. Obviously this process can't be implemented since the defect insertion is possible only during the sheet growth. Presence of the defect in graphene layer means the deformation of the whole layer structure – the layer is not flat even in areas far from the defect (Fig. 6) [2].

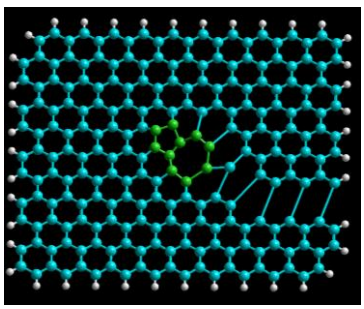


Fig. 5. 5-7 line defect.

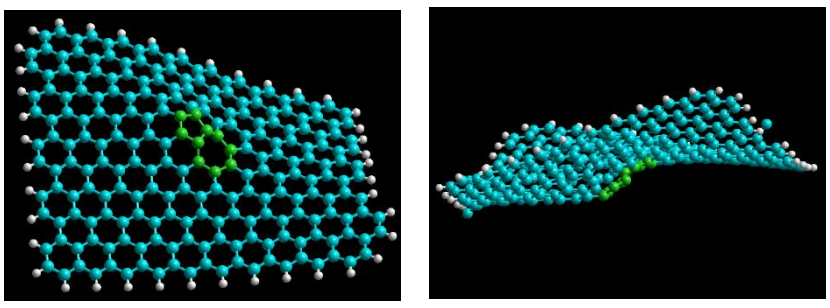


Fig. 6. 5-7 line defect after structure geometric optimization.

Nanotubes with simple penta- and heptagon topological defects were formed by twisting graphene sheet with corresponding defect into a tube. Then the tube is completed by connecting 10x10 carbon nanotube. As a result new carbon nanotubes depicted in Figs. 7 and 8 are formed.

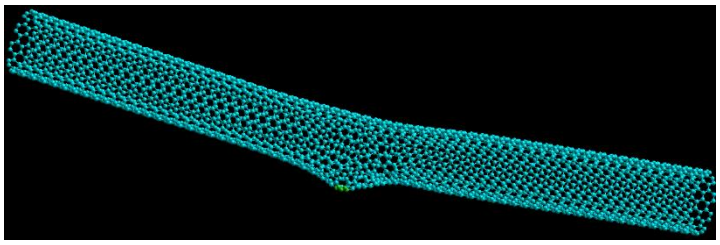


Fig. 7. The structure of carbon nanotube with simple pentagon topological defect.

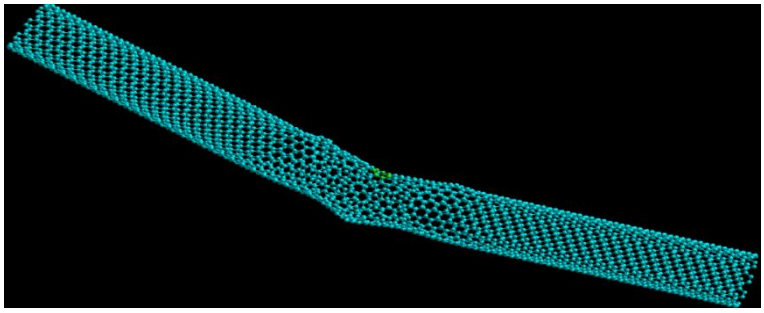


Fig. 8. The structure of carbon nanotube with simple heptagon topological defect.

3. Computer-aided atomic-molecular modelling of defective graphene structures

Graphen fragments with simple pentagon and heptagon topological defects and 30 and 42 boundary atoms correspondingly were prepared by atom-to-atom building (Fig. 9) for using in MATLAB home-made application program.

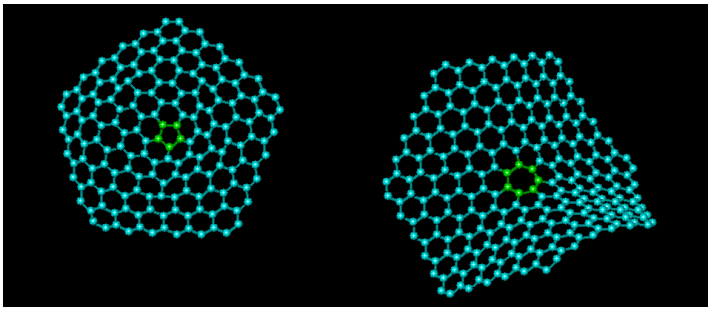


Fig. 9. Fragment of graphene layer with simple pentagon and heptagon topological defect.

First of all in this program the square graphene layer was constructed containing 15 atom per side (Fig. 10).

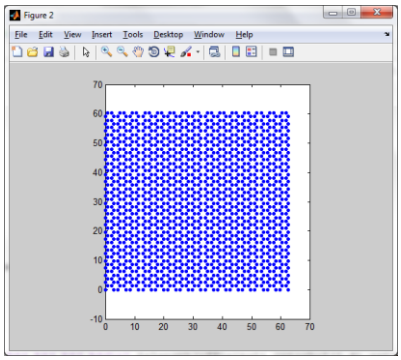
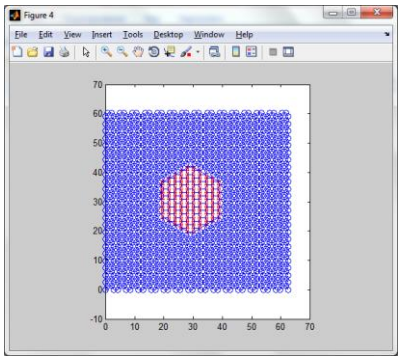


Fig. 10. 15x15 graphene layer.



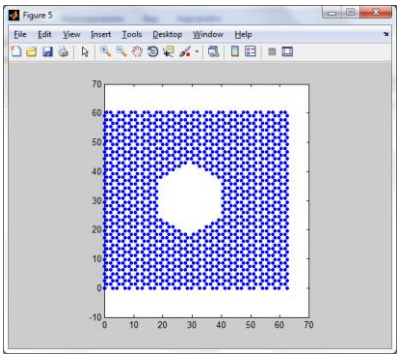


Fig. 11. Removal of graphene layer atoms.

The heptagon fragment containing 30 or 42 boundary atoms was then removed from the graphene fragment in accordance with number of boundary atoms in fragments under inserting (Fig. 11).

After new fragment insertion into vacant area and its bonding with the graphene part at rest the graphene with simple pentagon or heptagon topological defect is formed (Fig. 12 for pentagon). It is to be noted that 4 extra pentagons and 5 extra heptagons are formed for pentagon defect and vice-versa for heptagon one. This is the only way of defective graphene sheet localization of deformation.

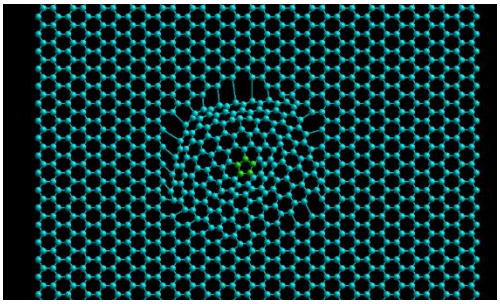


Fig. 12. Resulting graphene layer with defect.

After optimization, the graphene layer with inserted pentagon buckles as depicted in Fig. 13.

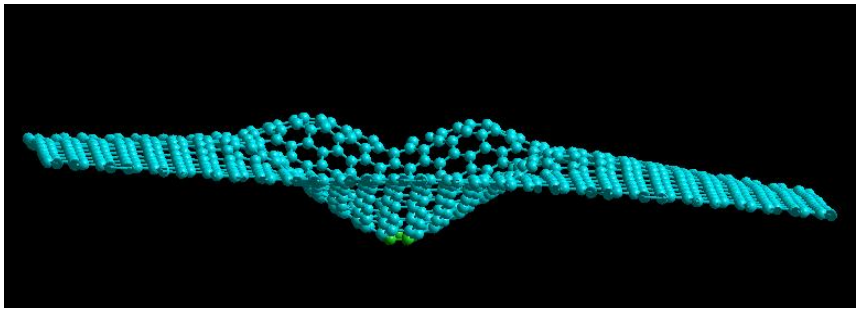


Fig. 13. Resulting graphene layer after optimization.

Localized insertion of the fragment with heptagon is carried out in the same way.

4. Conclusion

Analysis of possible ways of complex defect insertion into ideal graphene sheet revealed that the mechanism depends on the defect type (line or spot). Deformation degree of the graphene sheet structure depends on defects localization towards each other and combination of topological defects inserted into it.

Research of graphene layer topological defects is of interest since the defects significantly affect electronic, mechanical and elastic properties of carbon nanostructures.

References

[1] EA Belenkov, Y. Gizatullina, *Topological defects in graphene layers* (Scientific Library of Chelyabinsk State University, Chelyabinsk, 2010), p. 32. (In Russian).

[2] T.I. Grigorenko, In: *Collection of scientific papers based on student scientific and technical conferences of Mechanical Engineering Faculty* (Belarusian National Technical University, Minsk, 2014), p. 9. (In Russian).