Supracrystalline nanoribbons for nanoelectronics

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Abstract.
In the last two decades various forms of carbon nanostructures have attracted a great deal of interest due to their novel fundamental properties and possible applications in electronics. With the developments in production methods, these materials have emerged as one of the most promising materials for non-silicon electronics. Among carbon nanostructures graphene is a flat monolayer of carbon atoms tightly packed into a 2-D honeycomb lattice and is considered as the basic building block of other graphitic materials in all dimensions [1].

In the past, 2-D materials were thought to be thermodynamically unstable and could not exist. In 2004, experimental discovery of graphene showed that these materials can exist in liquid suspensions or on non-crystalline substrates. Because of this fact, theoretical studies on graphite are much more than experimental ones.

The possibility of more complicated than graphene two-dimensional periodic structures existence has been theoretically proved. There are not separate atoms or ions but its symmetric complexes at the nodes at their crystalline lattice [2]. They were called as supracrystals.

1. Materials and methods
Since graphene is a semimetal, it’s impossible to save from carriers in it when gate voltage applied, and therefore there will always be a high leakage current in graphene structures. To overcome this undesirable effect it is suggested to use narrow strips of graphene, because of the size called nanoribbons, where a formation of the band gap is possible because of the quantum size effect, and the width of the band gap is inversely proportional to transverse size of the ribbons. When defects appear on the border the nanoribbons change their state from the metallic to the semiconducting state.

Theoretically proved the possibility of the existence of more complex than graphene, 2D-carbon nets of sp2-hybridized carbon atoms forming the structure consisting of 3- and 12-polygons, 4-, 6- and 12-polygons. They can be considered as two-dimensional crystals formed by square or hexagonal cells with junctions consisted of proper atomic (or ionic) polygons but not separate atoms or ions. Such structures were called 2D-supracrystals [2].

The letters X and Y in brackets determine the chemical element symbol in indications of supracells in 2D- supracrystals (Fig. 1). The indexes after these letters mean: the first index defines the type of supracell, the next indexes describe the types of the cells enclosed. Firstly, the number of sides of the junction cells, then the number of sides of the surrounding cells (if they exist).
2. The results of modeling and calculations.

With the help of a software package NanoEngineer supracrystalline nanoribbons were modeled and tested for stability which are obtained by various methods of cutting. Various types of nanoribbons (C)$_{44}$ are shown in Fig. 2.
Figure 2. Supracrystalline sheets and various tapes of nanoribbons (X). The ribbons that can be rolled into nanotubes are marked by the letters NT [3].

The method of molecular dynamics was chosen to give a theoretical appreciation of band gap for graphene and supracrystal nanoribbons, as it requires the least computer resources. The fundamental principles of molecular dynamics and particle dynamics are based on twin charges of Lennard-Jones interactions. The idea of a twin charge means that the interaction of two particles depends on their relative positions and does not depend on the positions of any other particles. All Lennard-Jones charges describe the interactions where repulsions are typical for smaller distances and attractions for greater distances. The Lennard-Jones charges allow to describe properly many physical phenomena and properties of substances on a high-quality level.

The graphs are showing the results of calculations of the band gap of the «zig-zag» (Fig.5) and «armchair» (Fig.6) graphene nanoribbons and supracrystal (C)$_{44}$ (Fig.3) and (Si)$_{44}$ nanoribbons, depending on the width of the nanoribbons.
Figure 3. The dependence of the band gap supracrystal nanoribbon \((C)_{44} L = 23.68 \text{ nm}\) from the width of the ribbon.

Figure 4. The dependence of the band gap supracrystal nanoribbon \((Si)_{44} L = 24.67 \text{ nm}\) from the width of the ribbon.

Figure 5. The dependence of the band gap of graphene nanoribbons with the edges of the "zig-zag" type \(L = 21.73 \text{ nm}\) from the width of the ribbon.
3. Conclusions

The variations of the boundary conditions, chemical composition and chirality permit to obtain the supracrystalline nanoribbons with different electrical characteristics which are of interest for practical applications. In this work we present the results of simulation and calculations of energy stability and electrical characteristics (band gap) for supracrystalline nanoribbons of different symmetry made on the base of C, Si, S, B-N. We have demonstrated, that such nanoribbons may be successfully used in nanoelectronics.

References
1. Novoselov K. S. et al. Two-dimensional atomic crystals // PNAS. 2005. V. 102. P. 10451.
2. Brazhe R.A., Karenin A.A. Simulation of the supracrystal’s physical properties // Izvestia VUZOV. Povolzhskii region. Fiziko-matematicheskie nauki. 2011. 17 (1).
3. Arefeva P.A., Brazhe R.A., Karenin A.A. Supracrystalline nanoribbons // Radioelektronnaya technika. Ulyanovsk, 2010. P. 141-147.