ISSN 1561-2430 (Print)
ISSN 2524-2415 (Online)

ФИЗИКА

PHYSICS

UDC 539.21
https://doi.org/10.29235/1561-2430-2020-56-4-411-418

Received 13.11.2020
Поступила в редакцию 13.11.2020

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THE GEOMETRY OF A BILAYER NANOSCROLL ROLLED FROM ZIGZAG NANORIBBONS OF GRAPHENE AND BORON NITRIDE

Abstract. Herein, an algorithm is proposed for calculating the Cartesian coordinates of a bilayer nanoscroll rolled from a zigzag graphene nanoribbon (*n*zGNR) and a commensurate boron nitride nanoribbon (*n*zBNNR) into two Archimedean spirals. The distance between the layers and the inner radius of the nanoscroll, the length and width of *n*zGNR, and the length of the chemical bond between the atoms in the ribbon are the parameters used in the algorithm. It is assumed that these parameters are equal both for *n*zGNR and *n*zBNNR.

Keywords: graphene, boron nitride, Cartesian coordinates, nanoribbon, bilayer nanoscroll

For citation. Poklonski N. A., Siahlo A. I., Vyrko S. A., Ratkevich S. V., Vlassov A. T., Lozovik Yu. E., Hieu N. N. The geometry of a bilayer nanoscroll rolled from zigzag nanoribbons of graphene and boron nitride. *Vestsi Natsyianal'nai akademii navuk Belarusi. Seryia fizika-matematychnykh navuk = Proceedings of the National Academy of Sciences of Belarus. Physics and Mathematics series*, 2020, vol. 56, no. 4, pp. 411–418. https://doi.org/10.29235/1561-2430-2020-56-4-411-418

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ГЕОМЕТРИЯ ДВУХСЛОЙНОГО НАНОРУЛОНА ИЗ ZIGZAG НАНОПОЛОСОК ГРАФЕНА И НИТРИДА БОРА

Аннотация. Предложен алгоритм вычисления декартовых координат двухслойного нанорулона, свернутого из зигзагообразной графеновой нанополоски (*n*zGNR) и соразмерной нанополоски нитрида бора (*n*zBNNR) в две архимедовы спирали. Используемые в алгоритме параметры: расстояние между слоями и внутренний радиус нанорулона, длина и ширина *n*zGNR, длина химической связи между атомами в нанополоске (для *n*zGNR и *n*zBNNR они приняты равными).

Ключевые слова: графен, нитрид бора, декартовы координаты, нанополоска, двухслойный нанорулон

Для цитирования. Геометрия двухслойного нанорулона из zigzag нанополосок графена и нитрида бора / Н. А. Поклонский [и др.] // Вес. Нац. акад. навук Беларусі. Сер. фіз.-мат. навук. – 2020. – Т. 56, № 4. – С. 411–418 (in English). https://doi.org/10.29235/1561-2430-2020-56-4-411-418

Introduction. A bilayer nanoscroll consists of two fragments of graphene or boron nitride rolled into one scroll [1, 2]. It is known that the energy and electromechanical characteristics of a system of not too many atoms can be calculated by quantum chemical methods [3, 4]. Software packages that implement quantum chemical calculations require specifying the starting positions (coordinates) of the atoms that make up the system. When starting a study of new objects such as nanoscrolls using methods of computational chemistry [5], the researcher is faced with a need to algorithmize [6] the calculation of the atomic coordinates of the starting configuration [7] of the object under study according to the given parameters. Currently, algorithms for calculating the coordinates of atoms in nanoscrolls are not available. In this regard, we note work [8], in which an algorithm was proposed for calculating the coordinates of atoms in a single-layer carbon nanoscroll rolled from a *zigzag* graphene nanoribbon (zGNR) without preserving the lengths of C–C bonds.

The purpose of the present work is to propose an algorithm for calculating the coordinates of atoms in a bilayer nanoscroll from commensurate *zigzag* nanoribbons of graphene and boron nitride (Gr/BN) based on a small number of parameters while maintaining the lengths of interatomic bonds $a_{CC} = a_{BN}$ in the nanoscroll.

The nanoscroll is a spiral cylindrical surface. Cylindricity is associated with the fact known from differential geometry [9, 10] that a cylindrical surface is isometric to a plane. The coils of the nanoscroll tend to unfold and become flat, but the nanoscroll is stable in such a folded state due to the van der Waals attraction of the layers [11, 12]. The distance between layers is determined by the interaction of atoms of the neighboring layers and should approximately be the same. It is known that the distance between the coils of the Archimedean spiral is also approximately the same. Therefore, the layers of the nanoscroll in the cross section approximately give an Archimedean spiral. This determines the geometry of nanoscrolls.

On the nanoribbon the coordinate system (X, Y) is selected (length along the X axis and width along the Y axis), while for a cylindrical surface in the $\mathbf{R}^3$ space the Cartesian coordinate system (x, y, z), the z axis being directed along the cylinder axis, together with a cylindrical coordinate system (r, φ, z) with polar coordinates in the xy plane are used. The unit vectors to the coordinate axes r, φ, and z will be denoted by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{k}$, respectively. The curve along which the surface bends is given in the xy plane in polar coordinates (r, φ) by the equation $\mathbf{r} = f(\varphi)\,\mathbf{e}_1(\varphi) = s\varphi(X)\,\mathbf{e}_1(\varphi)$, and the isometric mapping of the nanoribbon to the surface by the equation $\mathbf{r} = s\varphi(X)\,\mathbf{e}_1(\varphi) + y\mathbf{k}$.

The mathematical basis of the proposed constructions is the existence of an isometric map of a nanoribbon onto a cylindrical spiral surface: $(X, Y) \to (x, y, z) = (s\varphi(X), \varphi(X), Y)$. The nanoribbons under consideration are the fragments of two-dimensional crystals, on the nodes of which a translation group acts (locally). Due to the incompleteness of the nanoribbon, this is a local action. Isometry makes it possible to transfer the action of this group from the nanoribbon to the surface and to restore the lattice there using transformations of the group of a two-dimensional crystal lattice (see, e.g., [13]).

Atomic coordinates in nanoribbons. Figure 1 shows the structures of a flat carbon nanoribbon 46zGNR (*a*) and a bilayer Gr/BN nanoscroll (*b*) with an inner radius R_{in} of 1 nm, rolled from graphene and boron nitride nanoribbons in the form of two cylindrical surfaces formed by Archimedean spirals.

The length of a *zigzag* graphene nanoribbon *n*zGNR, from which the nanoscroll is rolled, is $L = (3n/2 - 1)a_{CC}$, where n is the number of *zigzag* chains along the length of the ribbon (along the X axis in Fig. 1, *a*), $a_{CC} = 0.142$ nm is the distance between the nearest carbon atoms. Thus, for the 46zGNR carbon nanoribbon ($n = 46$), the length L is 9.66 nm. The length of a commensurate nanoribbon of boron nitride 46zBNNR with the number of *zigzag* chains is $L = (3n/2 - 1)a_{BN}$. We assume that the distance between neighboring B and N atoms in a flat boron nitride nanoribbon is equal to the distance between neighboring carbon atoms in a flat graphene nanoribbon, i.e., $a_{BN} = a_{CC}$.

The atomic coordinates of the flat *zigzag* bilayer nanoribbon are determined by four indices (Fig. 1, *a*): the index q takes the values A and B or B and N and corresponds to two atoms in the unit cell of *n*zGNR or *n*zBNNR, the index i is the number of the unit cell along the length of the ribbon L, the index j is the number of the unit cell along the width of the ribbon W, and the index k is the number of the layer. The coordinates of the bilayer atoms in the AA configuration (when the X, Y coordinates of the atoms in both layers coincide) are given by the formulas:

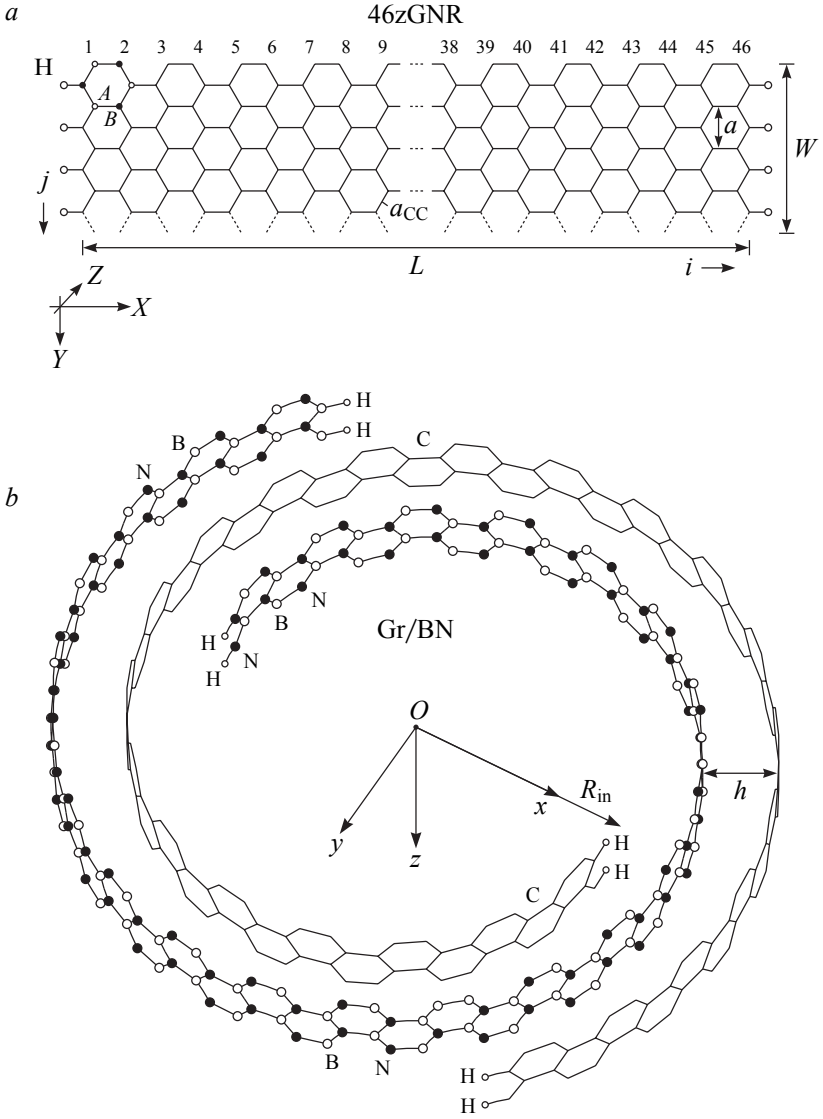

Fig. 1. The structure of a computational cell of width W for a flat 46zGNR nanoribbon of length L (*a*) and for a Gr/BN bilayer nanoscroll with the inner radius R_{in} = 1 nm (*b*). Here n = 46 *zigzag* chains of carbon atoms constituting 46zGNR are enumerated; $a_{CC} = a_{BN}$ is the bond length in the graphene and boron nitride nanoribbons, a is the translation period, and h is the distance between the layers (nanoribbons); the z axis is directed along the nanoscroll

$$
\begin{aligned}
&X_{Aij1} = (3/2)(i-1)a_{CC}, \quad X_{Bij1} = X_{Aij1} + a_{CC},\\
&X_{Bij2} = (3/2)(i-1)a_{BN}, \quad X_{Nij2} = X_{Nij2} + a_{BN},\\
&Y_{qijk} = (j-1)a + a/2 \quad \text{for odd } i,\\
&Y_{qijk} = (j-1)a \quad \text{for even } i,\\
&Z_{qijk} = (k-1)h,
\end{aligned} \tag{1}
$$

where $a = \sqrt{3}\, a_{CC}$ is the translation period of the bilayer (along the Y axis) and h = 0.335 nm is the distance between the layers.

The free *zigzag* edges of both nanoribbons are passivated by hydrogen atoms located at a distance of a_{CH} = 0.1091 nm from carbon atoms along the X axis in *n*zGNR, and a_{BH} = 0.119 nm from boron and a_{NH} = 0.1008 nm from nitrogen atoms in *n*zBNNR.

Atomic coordinates in nanoscrolls. Two nanoribbons of graphene and boron nitride, rolled around an axis perpendicular to the length of the ribbon (around the y axis in Fig. 1, *a*), form the bilayer Gr/BN nanoscroll, as shown in Fig. 1, *b*. (Note that the bilayer nanoscroll can also be rolled from a graphene

and boron nitride bilayer when the initial angular coordinates of the layers coincide.) The cross section of the nanoscroll is two Archimedean spirals with a distance between the adjacent layers $h = 0.335$ nm. Each atom is characterized by four indices: q corresponds to two atoms in the unit cell of graphene (takes the values A and B or B and N for the boron nitride unit cell); i is the number of the unit cell of graphene along the length L (from 1 to n_L); j is the number of the unit cell of graphene along the width (from 1 to n_W); and k is the layer number for a multilayer nanoscroll (from 1 to n_h). For the bilayer nanoscroll made of graphene and boron nitride, we assume $k = 1$ for the graphene layer and $k = n_h = 2$ for the boron nitride layer. The Cartesian coordinates of nanoscroll atoms $(x_{qijk}, y_{qijk}, z_{qijk})$ through the cylindrical coordinates $(R_{qijk}, \varphi_{qijk}, z_{qijk})$ are represented as follows:

$$\begin{aligned} &x_{qijk} = R_{qijk}\cos(\varphi_{qijk}), \quad y_{qijk} = R_{qijk}\sin(\varphi_{qijk}),\\ &z_{qijk} = (j-1)a + a/2 \quad \text{for odd } i,\\ &z_{qijk} = (j-1)a \quad \text{for even } i, \end{aligned} \tag{2}$$

where $R_{qijk} = n_h h\varphi_{qij1}/2\pi$ is the polar radius of the nanoscroll atom corresponding to the angle $\varphi_{qijk} = \varphi_{qij1} + (k-1)2\pi/n_h$ in the layer with number k, and $a = \sqrt{3}\,a_{CC}$ is the scroll translation period along the z axis. Note that we use different coordinate systems for the nanoscroll and nanoribbons. For nanoribbon, the X axis is directed along its length L, and for the nanoscroll, the xy plane is perpendicular to its axis. Let us consider two methods for finding the unknown angle φ_{qij1}.

The first method. Let us consider an approximate method for describing a nanoscroll, when the distances between atoms in a flat nanoribbon are equal to the distances on a curved surface bent along an Archimedean spiral (isometric mapping of a nanoribbon onto a cylindrical surface). In this case, the distances between neighboring atoms in the nanoscroll are not equal to the interatomic distances a_{CC} in flat nanoribbons (Fig. 1). The unknown angle φ_{qij1} is found from the equation $X_{qij1} = \Lambda(\varphi_{in}, \varphi_{qij1})$, where X_{Aij1} $(= X_{Bij2}) = (3/2)(i-1)a_{CC}$, X_{Bij1} $(= X_{Nij2}) = X_{Aij1} + a_{CC}$ are the coordinates of atoms in the graphene (and boron nitride) layer along the X axis of the corresponding flat nanoribbon (see also Eq. (1)), $\Lambda(\varphi_{in}, \varphi_{qij1})$ is the length of the Archimedean spiral with a helix pitch distance $n_h h$, an initial angle φ_{in}, and a final angle φ_{qij1}.

$$\Lambda(\varphi_{in}, \varphi_{qij1}) = \int_{\varphi_{in}}^{\varphi_{qij1}} \frac{n_h h}{2\pi}\sqrt{1+\varphi^2}\,d\varphi = \frac{n_h h}{4\pi}\Big[\varphi_{qij1}\sqrt{1+\varphi_{qij1}^2} - \varphi_{in}\sqrt{1+\varphi_{in}^2} +$$

$$+\ln\left(\varphi_{qij1} + \sqrt{1+\varphi_{qij1}^2}\right) - \ln\left(\varphi_{in} + \sqrt{1+\varphi_{in}^2}\right)\Big]. \tag{3}$$

The initial angle φ_{in} of a nanoscroll is expressed through the inner radius R_{in} as follows: $\varphi_{in} = 2\pi R_{in}/n_h h + (k-1)2\pi/n_h$. Expression (3) for the length of the spiral at angles large enough, compared to unity, can be approximately written in the form:

$$\Lambda(\varphi_{in}, \varphi_{qij1}) \approx \frac{n_h h}{4\pi}\left(\varphi_{qij1}^2 - \varphi_{in}^2\right). \tag{4}$$

Approximate relation (4) for the spiral length $\Lambda(\varphi_{in}, \varphi_{qij1})$ allows us to analytically solve the equation $X_{qij1} = \Lambda(\varphi_{in}, \varphi_{qij1})$ with respect to the unknown angle:

$$\varphi_{qij1} = \sqrt{4\pi X_{qij1}/n_h h + \varphi_{in}^2}\,.$$

In order to start the nanoscroll from a zero angle in cylindrical coordinates (correspondingly from the x axis in Cartesian coordinates), the Archimedean spiral can be represented in the form: $R_{qijk} = R_{in} + n_h h(\varphi_{qij1} - \varphi_0)/2\pi$, where $\varphi_0 = 2\pi R_{in}/n_h h$ and parameter $n_h = 2$ for a bilayer nanoscroll. Thus, the Cartesian coordinates (x_{qijk}, y_{qijk}) in Eq. (2) can be rewritten as follows: $x_{qijk} = R_{qijk}\cos(\varphi_{qijk} - \varphi_0)$, $y_{qijk} = R_{qijk}\sin(\varphi_{qijk} - \varphi_0)$.

The second method. In some cases, it may be necessary to take into account the difference between the arc and chord lengths on the spiral surface of the nanoscroll. This difference depends on the curvature K of the surface, which at the point with the current radius $r = s\varphi$ is [10, 14]:

$$K(r) = \frac{r^2 + 2s^2}{(r^2 + s^2)^{3/2}}.$$

If $r \gg s$, then the curvature of the Archimedean spiral is $K \approx 1/r$, as for a circle of radius r. For a circle, the difference between the length of the chord l and the length of the corresponding arc D is of the third order by D, namely $D^3/24r^2$. Indeed, the length of the chord $l = 2r\sin(\Delta\varphi/2)$, the length of the arc $D = r\Delta\varphi$, expanding into a series in powers of $\Delta\varphi$, we obtain $l \approx r\Delta\varphi - r(\Delta\varphi)^3/24 = D - D(\Delta\varphi)^2/24$, i.e., $D - l \approx D(\Delta\varphi)^2/24 = D^3/24r^2$. Then the difference between the lengths of the spiral and the n-chord spiral on one turn can be estimated as $n(D - l) \approx nD(D^2/24r^2) = 2\pi r(D^2/24r^2) \approx 2\pi r(l^2/24r^2)$.

Now we select the mapping of a nanoribbon to a nanoscroll, in which the distances between neighboring atoms in the nanoscroll are equal to the distances $a_{CC} = a_{BN}$ in flat ribbons. Let there be two points on the plane $A = (X_0, Y_0)$ and $B = (X_1, Y_1)$ related to neighboring atoms. The mapping onto a cylindrical surface is given by the formula:

$$(X, Y) \to (x, y, z) = \big(r(\varphi)\cos(\varphi),\, r(\varphi)\sin(\varphi),\, Y\big).$$

The surface is constructed along the spiral $r(\varphi) = s\varphi$, where $s = n_h h/2\pi$. Points A and B transfer to the following points, respectively

$$A' = \big(r(\varphi_0)\cos(\varphi_0), r(\varphi_0)\sin(\varphi_0), Y_0\big),$$
$$B' = \big(r(\varphi_1)\cos(\varphi_1), r(\varphi_1)\sin(\varphi_1), Y_1\big).$$

Let the angle φ_0 be known for the point A' and we need to determine φ_1. Let us find the angle φ_1 for the point B' from the equality of the distances between the original points and their images: $|AB| = |A'B'|$. Transforming the left and the right sides of this equation in accordance with the Pythagorean theorem, we have

$$|A'B'|^2 = \big(r(\varphi_1)\cos\varphi_1 - r(\varphi_0)\cos\varphi_0\big)^2 + \big(r(\varphi_1)\sin\varphi_1 - r(\varphi_0)\sin\varphi_0\big)^2 + (Y_1 - Y_0)^2,$$
$$|AB|^2 = (X_1 - X_0)^2 + (Y_1 - Y_0)^2.$$

Equating the right-hand sides, we get

$$(X_1 - X_0)^2 = r^2(\varphi_1) + r^2(\varphi_0) - 2r(\varphi_1)r(\varphi_0)\cos(\varphi_1 - \varphi_0). \tag{5}$$

This relation is the law of cosines for the length $|A'B'|$ of a spiral chord (Fig. 2).

To implement this folding method, it is necessary to transform the indexing of X_{qij1} coordinates over the first two indices q, i into one "doubled" index p, which is sequentially run through the atoms in the jth *armchair* chain (Fig. 1, *a*).

Using Eq. (5), we write the equation for the desired angle $\varphi_{(p+1)j1}$ from the known angle φ_{pj1} while maintaining the interatomic distances:

$$\big(X_{(p+1)j1} - X_{pj1}\big)^2 = (n_h h/2\pi)^2\big[(\varphi_{(p+1)j1})^2 + (\varphi_{pj1})^2 - 2\varphi_{(p+1)j1}\varphi_{pj1}\cos(\varphi_{(p+1)j1} - \varphi_{pj1})\big], \tag{6}$$

where $\varphi_{1j1} = 2\pi R_{in}/n_h h$ is the initial angle of the spiral.

Equation (6) is nonlinear and can be solved numerically. Since the cosine is an even periodic function, you should take guess values of the angles close to the desired ones, otherwise the numerical solution method can find roots with negative angles or roots that differ from the desired ones by a multiple of 2π. It is convenient to take the following approximate values as the guess values:

$$\varphi_{(p+1)j1} = \sqrt{(4\pi/n_h h)X_{(p+1)j1} + \varphi_{in}^2},$$

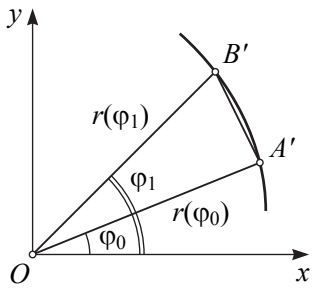

Fig. 2. On the determination of the length of the spiral chord $|A'B'|$ from the law of cosines

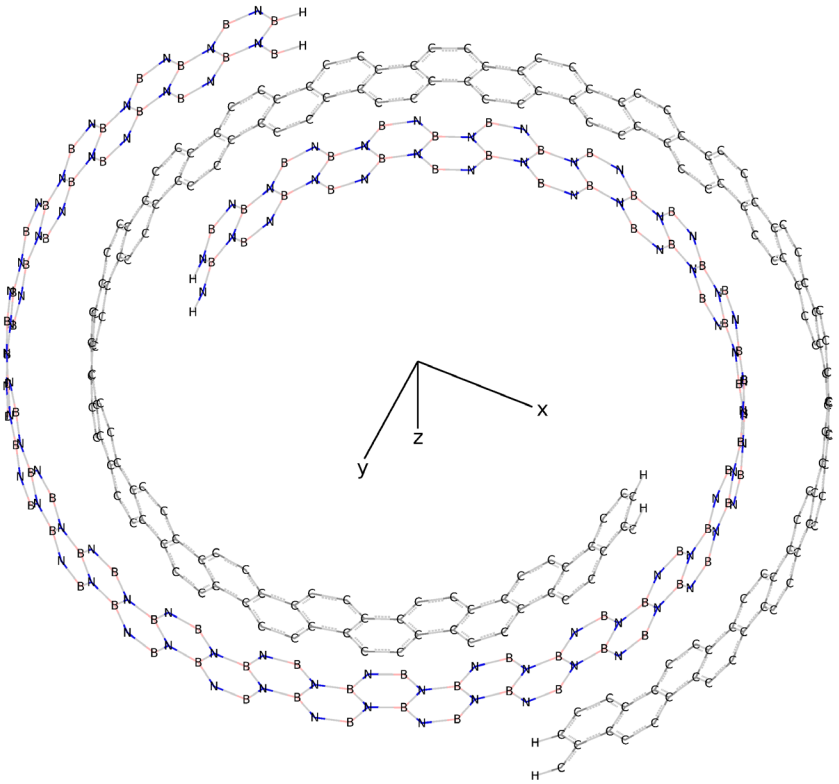

Fig. 3. A computational cell for a bilayer Gr/BN nanoscroll rolled from a 46zGNR graphene nanoribbon and a commensurate 46zBNNR boron nitride nanoribbon with the inner radius R_{in} = 1 nm displayed in the graphical interface GaussView; the z axis of the Cartesian coordinate system is directed along the nanoscroll

found from Eq. (4). Or even simpler (approximating spiral arcs by circular arcs of the corresponding radius):

$$\varphi_{(p+1)j1} = \varphi_{pj1} + \left[\left(X_{(p+1)j1} - X_{pj1}\right)/r(\varphi_{pj1})\right].$$

The Cartesian coordinates of a bilayer Gr/BN nanoscroll with equal bond lengths $a_{CC} = a_{BN}$ obtained using the proposed algorithm are suitable for use in standard software packages for quantum chemical calculations (Fig. 3). The data to reproduce these findings are available to download [15].

Conclusion. An algorithm for calculating the Cartesian coordinates of the atoms of a bilayer nanoscroll in the form of two Archimedean spirals is proposed. The length and width of the graphene and boron nitride nanoribbons, the distance between adjacent layers, the inner radius of the nanoscroll, and the distance between neighboring atoms in flat *zigzag* nanoribbons are the parameters defining the nanoscroll. The starting configurations of nanoscrolls with equal bond lengths, folded from *zigzag* nanoribbons of graphene and boron nitride, are constructed, which are suitable for calculating the parameters of nanoscrolls by quantum chemical methods.

Acknowledgements. The work was supported by the Belarusian National Research Program "Convergence-2020" and the Belarusian Republican Foundation for Fundamental Research (grant no. Ф20Р-301). Yurii E. Lozovik acknowledge support by the Russian Foundation of Basic Research (grant no. 20-52-00035) and the Program for Basic Research of the National Research University "Higher School of Economics". Nguyen Ngoc Hieu acknowledge support by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant no. 103.01-2017.309.

Благодарности. Работа поддержана Государственной программой научных исследований «Конвергенция-2020» Республики Беларусь и Белорусским республиканским фондом фундаментальных исследований (грант № Ф20Р-301). Ю. Е. Лозовик благодарит за поддержку Российский фонд фундаментальных исследований (грант № 20-52-00035) и Программу фундаментальных исследований Национального исследовательского института «Высшая школа экономики». Нгуен Нгок Хиеу благодарит за поддержку Вьетнамский национальный фонд развития науки и технологий (NAFOSTED) в рамках гранта № 103.01-2017.309.

References

1. Siahlo A. I., Poklonski N. A., Lebedev A. V., Lebedeva I. V., Popov A. M., Vyrko S. A., Knizhnik A. A., Lozovik Yu. E. Structure and energetics of carbon, hexagonal boron nitride, and carbon/hexagonal boron nitride single-layer and bilayer nanoscrolls. *Physical Review Materials*, 2018, vol. 2, no. 3, pp. 036001 (1–9). https://doi.org/10.1103/PhysRevMaterials.2.036001

2. Perim E., Galvão D. S. The structure and dynamics of boron nitride nanoscrolls. *Nanotechnology*, 2009, vol. 20, no. 33, pp. 335702 (1–6). https://doi.org/10.1088/0957-4484/20/33/335702

3. Lewars E. G. *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*. Berlin, Springer, 2016. xvi+728 p. https://doi.org/10.1007/978-3-319-30916-3

4. Poklonski N. A., Vyrko S. A., Siahlo A. I., Poklonskaya O. N., Ratkevich S. V., Hieu N. N., Kocherzhenko A. A. Synergy of physical properties of low-dimensional carbon-based systems for nanoscale device design. *Materials Research Express*, 2019, vol. 6, no. 4, pp. 042002 (1–25). https://doi.org/10.1088/2053-1591/aaf b1c

5. Cramer C. J. *Essentials of Computational Chemistry: Theories and Models*. Chichester, Wiley, 2004. xxii+596 p.

6. Cormen T. H., Leiserson C. E., Rivest R. L., Stein C. *Introduction to Algorithms*. Cambridge, MIT Press, 2009. xx+1292 p.

7. Brázdová V., Bowler D. R. *Atomistic Computer Simulations: A Practical Guide*. Weinheim, Wiley-VCH, 2013. xxx+332 p. https://doi.org/10.1002/9783527671816

8. Siahlo A. I., Vyrko S. A., Ratkevich S. V., Poklonski N. A., Vlassov A. T., Hieu N. N., Lozovik Yu. E. Quantum chemical calculations of carbon nanoscroll energy rolled from zigzag graphene nanoribbon. *Semiconductors*, 2020, vol. 54, no. 12, pp. 1678–1681. https://doi.org/10.1134/s1063782620120350

9. Rashevskii P. K. *Course of Differential Geometry*. Moscow, GITTL, 1956. 420 p. (in Russian).

10. Kühnel W. *Differential Geometry: Curves, Surfaces, Manifolds*. Providence, AMS, 2015. xii+402 p.

11. Yankowitz M., Ma Q., Jarillo-Herrero P., LeRoy B. J. van der Waals heterostructures combining graphene and hexagonal boron nitride. *Nature Reviews Physics*, 2019, vol. 1, no. 2, pp. 112–125. https://doi.org/10.1038/s42254-018-0016-0

12. Galashev A. E., Rakhmanova O. R. Mechanical and thermal stability of graphene and graphene-based materials. *Physics Uspekhi*, 2014, vol. 57, no. 10, pp. 970–989. https://doi.org/10.3367/UFNe.0184.201410c.1045

13. Poklonski N. A., Vlassov A. T., Vyrko S. A. *Finite Symmetry Groups: Fundamentals and Applications*. Minsk, P. Brouka Belarusian Encyclopedia, 2011. 464 p. (in Russian).

14. Archimedean spiral. Prokhorov Yu. V. (ed.) *Mathematical Encyclopedic Dictionary.* Moscow, Sovetskaya entsiklopediya Publ., 1988. pp. 80 (in Russian).

15. Vyrko S. A., Siahlo A. I., Poklonski N. A., Vlassov A. T., Ratkevich S. V., Lozovik Yu. E., Hieu N. N. Data for: Geometry of bilayer nanoscroll rolled from zigzag nanoribbons of graphene and boron nitride. *Mendeley Data*. 2020. https://doi.org/10.17632/rz57w938fs

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