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CRYSTALLOGRAPHY OF COAXIAL AND SCROLL NANOTUBES OF ARBITRARY COMPOSITION

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Abstract. Cylindrical coordinates of atoms of multilayer nonchiral, chiral and scroll nanotubes of arbitrary composition are developed by projecting the structure of plane analogue on corresponding surface. The coaxial and spiral cylindrical lattices, Bravais cells and chiral indexes, expressed in terms of these cells, are used for description of nanotubes structure. The model of multilayer chiral nanotube with not close packed layers is proposed.

Keywords: nanotube, chiral, spiral, scroll.

1. Introduction

Nanotubes were first opened at the beginning of the 50-th by direct observation of the particles of chrysotile, garnierite and halloysite in electron microscope [1-3]; then the bases of nanotubes crystallography were founded as generalization of the traditional theory on cylindrical crystals [4-6]. The experimental researches have shown that nanotubes are of four basic types (Fig. 1): coaxial – circular (non-chiral) and chiral (helical), and spiral – roll (scroll) and cone (cone scroll), and also have polytype modifications, associated with mutual shifts and turns of layers. Today the nanotubes crystallography is at the beginning of its development, therefore there is a description of structure of three types of nanotubes only: circular, chiral and roll [7]. All known nanotubes have layer structure and plane analogues with the same structure of unit cell: carbon nanotube – graphite, chrysotile – lizardite, SnS_2-nanotube – stanisulite, *etc*. Therefore the nanotubes description is developed on the basis of structures of analogues in view of cylindrical symmetry. Let us consider some aspects of the problem, general for all types of nanotubes.

The nanotubes structure is expressed in cylindrical coordinate system $\{\rho, \varphi, z\}$ by projecting the analogue's layer structure on the corresponding surface (the axis z coincides with nanotubes axis). It allows using the structural data of analogue for the nanotube description. According to the rules accepted for layer crystals the Bravais cell parameters a and b are chosen in a plane of layer. The parameter c of cylindrical lattice is indefinite, the thickness of layer d, and also longitudinal and azimuthal interlayer shifts are used instead of it. The basis of nanotubes crystallography is expression for radiuses of their layers:

$$r_m = r_0 + md \qquad (1)$$

where ρ_0 – internal radius of nanotube, m = 0–M-1 – number of the layer, M – quantity of layers.

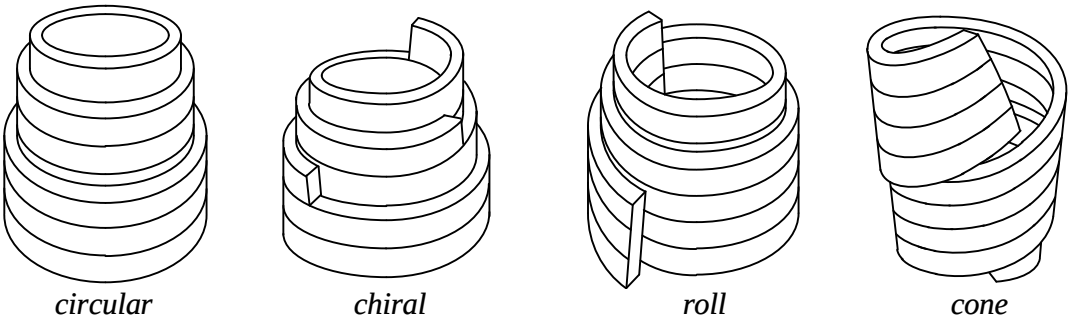


Fig. 1. The general types of nanotubes

At a cylindrical bend of layer the origin of Bravais cell in radial direction is chosen on the level on which the value of circular parameter b of cylindrical lattice does not depend on curvature of cell. For example, such level of cell of sulfide and chrysotile nanotubes coincides with a sheet of metal; in case of carbon nanotube the choice is obvious. Thus, the choice of nanotube cells origin in a radial direction is not arbitrary.

Availability of special direction – the nanotube axis – allows proposing a single axes selection for its structure description. Let us assume rectangular Bravais cell (Fig. 2) is formed by basic vectors: $\vec{a}$, closest to nanotube axis, and $\vec{b}$, closest to its cross section; at such axes selection the chiral angle ε_c is minimal. Let us set the atom position in a plane layer by vector $\vec{r}_{mj} = \vec{r}_m + \vec{r}_j$, where $\vec{r}_m = n\vec{a} + n\vec{b}$ – the plane lattice vector, n and v – integers, j – the number of atom in Bravais cell. Then vector $\vec{r}_j$, determining atom position in Bravais cell, has components x_j, y_j and z_j along vectors $\vec{a}$, $\vec{b}$ and lengthways the normal to layer, accordingly. Hence, vector $\vec{r}_{mj}$ has components: $an + x_j$ – in direction of vector $\vec{a}$, $bv + y_j$ – along vector $\vec{b}$ and z_j – lengthways the normal to layer. It is necessary to note that coordinate z_j may have any sign because of the special choice of cell's origin in the radial direction.

To transform coordinates in cylindrical system let us enter in the layer's plane two two-dimensional rectangular systems of coordinates {y', z'} and {y, z} (Fig. 2), having the same origin and turned respectively to each other on angle ε_c, thus the axis z is parallel to nanotube axis and axis y' – to vector $\vec{b}$. Then in the system {y', z'} atoms have coordinates: $y'_{nj} = bn + y_j$, $z'_{nj} = an + x_j$. The transformation of coordinates from system {y', z'} to system {y, z} gives:

$$\begin{cases} y_{mj} = (bn + y_j)\cos e_c - (an + x_j)\sin e_c \\ z_{mj} = (bn + y_j)\sin e_c + (an + x_j)\cos e_c \end{cases}. \qquad (2)$$

After discovering carbon nanotubes the alternative description of nanotubes structure was proposed, not using concepts "unit cell" and "cylindrical lattice" [8, 9]. Nanotube was built with the help of a set of helical lines, along which all atoms were located. This is equivalent to description of usual crystal as a set of sublattices which number is equal to number of atoms in unit cell. It is obvious that such approach complicates both the analysis of effects associated with local point symmetry, and use of the structural data of plane analogues. The way of definition of cylindrical layer with the help of pair integers (chiral indexes), proposed there, is rather convenient [10]. But the units (structural hexagons) in terms of which these numbers are expressed are not universal, as there is no firm belief that the layers of all nanotubes have hexagonal symmetry. Really, the mixed-layer nanotubes SnS_2/SnS [11] were synthesized recently, which SnS-layers have no structural hexagons and, hence, their chiral indexes cannot be determined. It is obvious that the chiral indexes expressed in terms of unit cells can be universal only.

As the axis z coincides with nanotube axis, the cylindrical coordinates of atom in system {ρ, φ, z} for circular, chiral and roll structures (Fig. 1) result by equating of value y_{nvj} to the length of appropriate curve's arch in cross section of nanotube.

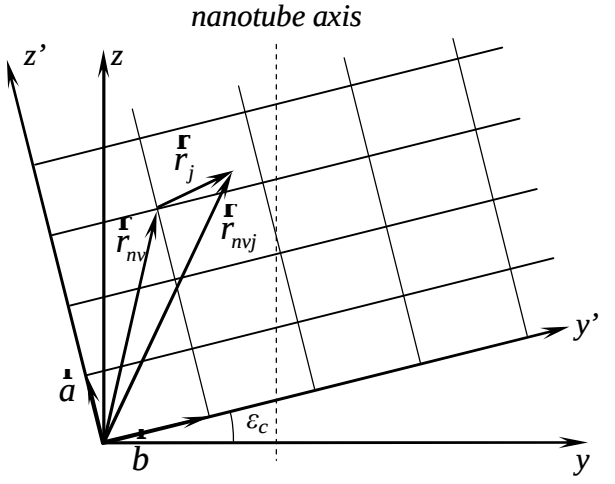


Fig. 2. The coordinate systems in layer, oriented respectively to nanotube axis

2. Circular Nanotube

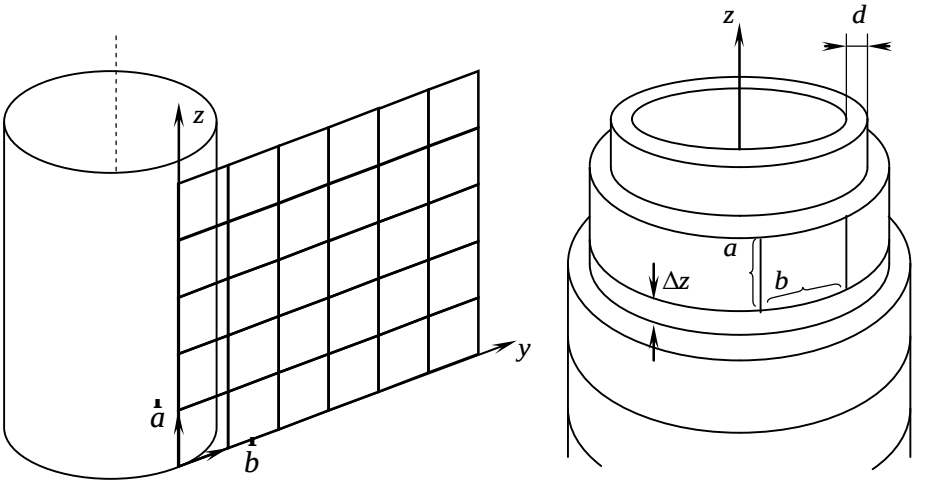
The structure of circular nanotubes is most simple, as a chiral angle $\varepsilon_c = 0$, therefore parameter a of Bravais cell is measured in direction of nanotube's axis, and parameter b – in direction of its cross section circle. The sites of cylindrical lattice are located on the site circles, which, in turn, are located on cylindrical surfaces (Fig. 3b). The atom coordinates (2) in system {y, z} become simpler:

$$\begin{cases} y_{nj} = bn + y_j \\ z_{nj} = an + x_j \end{cases} \qquad (3)$$

Limits of variation of integer parameters: n = 0–(N-1), v = 0–(p-1), where N – number of site circles on the cylinder, $p = 2\pi\rho/b$ – number of cells on the circle of cylinder, integer by definition.

In a case of multiwall circular nanotube taking into consideration (1) we get:

$$\begin{cases} r_{mj} = r_m + z_j = r_0 + md + z_j \\ j_{mj} = \dfrac{bn}{r_m} + \dfrac{y_j}{r_m} + e_m \\ z_{mnj} = an + x_j + \Delta z_m \end{cases} \qquad (5)$$



a) b)

Fig. 3. The projecting and parameters of the circular nanotube

where values ε_m and Δz_m determine the origin of m-th layer in azimuthal and longitudinal directions, accordingly, in relation to the general origin. As a matter of fact, these values define the mutual ordering of layers in these directions, and also the polytype modifications, formed by appropriate interlayer shifts. For example, Whittaker [5] believed angular phases of layers ε_m are absolutely random (Whittaker's model); the azimuthal ordered model was proposed later [12]. For example, the experimental researches of chrysotile nanotubes show that the most widespread polytype modifications are monoclinic (clinochrysotile, $\Delta z_m = m\Delta z$, Fig. 4) and orthogonal (orthochrysotile, $\Delta z_m = 0$) [12]. The radial ordering of multiwall circular nanotube layers depends on realizing of close packing condition (1) at integer numbers p_m of cells on the circles of every layer. Let's assume there is an integer number p_m of unit cells on a site circle of m-th layer $p_m = \frac{2pr_m}{b}$. Then the number of cells on a circle of the following layer is equal to:

$$p_{m+1} = \frac{2p(r_m + d)}{b} = \frac{2pr_m}{b} + \frac{2pd}{b} = p_m + g \qquad (6)$$

where $g = \frac{2pd}{b}$ – generator of cylindrical lattice [5, 12]. It is visible that when p_0 and generator are integers the numbers of cells on the circles of every layer are integers too, that is the close packed circular nanotube takes place. Thus the number p_m varies on the value of generator at transition from one cylinder to another: $p_m = p_0 + mg$.

The generator g is a number determined by the sizes of unit cell. This implies that the layer structures capable to ensure the integer generator by their parameters b and d, can form perfect enough circular nanotubes only (for example, the generators of chrysotile and carbon "armchair" nanotube are equal to 5 with high accuracy). In Fig. 5 the examples of cross sections of circular lattices with various values of generator are given.

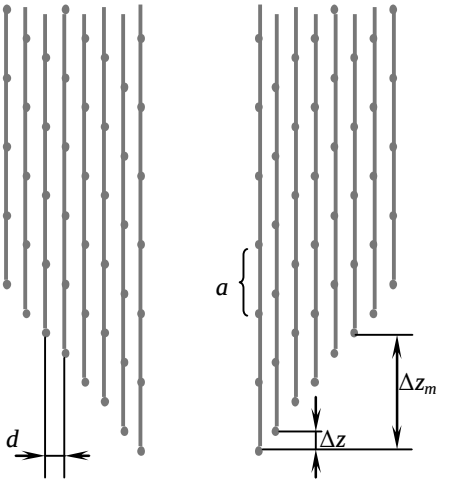
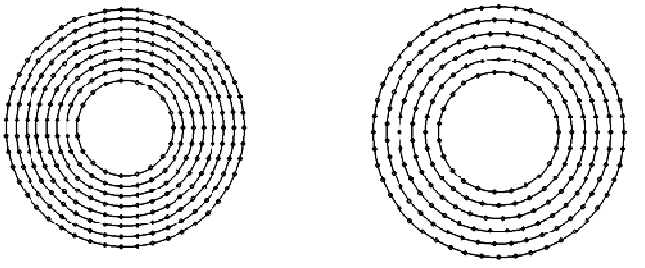


Fig. 4. The longitudinal section of monoclinic nanotube lattice



a) b)

Fig. 5. The cross-sections of circular lattices with $g = 4$ (a) and $g = 5$ (b)

3. Chiral Nanotube

In the case of singlewall chiral nanotube equating of coordinate y_{mj} to the length of circle arch in cross section (Fig. 6) according to (2) gives:

$$y_{mj} = r\,j \;\rightarrow$$

$$\rightarrow\; j_{mj} = \frac{1}{r}\left[\left(bn + y_j\right)\cos e_c - \left(an + x_j\right)\sin e_c\right] \qquad (7)$$

The expressions (2) and (7) determine z- and φ-coordinates of atoms, respectively, on a cylindrical surface with radius ρ. Thus the ρ-coordinate of atom is determined by condition $r_j = r + z_j$.

To form the regular singlewall chiral lattice it is necessary that the "end" of a layer was correctly combined with its "beginning", that is there should be an integer p of parameters b on a turn of site line (along vector $\vec{b}$ of a plan layer), and the step of this line (along vector $\vec{a}$ of a plan layer) should be equal to an integer s of parameters a. It means that (numbers of unit cells start from zero):

$$\begin{cases} j_{n,p,j} - 2p = j_{n+s,0,j} \\ z_{n,p,j} = z_{n+s,0,j} \end{cases} \qquad (8)$$

The substitution of (2) and (7) in (8) gives:

$$\mathrm{tg}\,e_c = \frac{as}{bp} \qquad r = \frac{1}{2p}\sqrt{(as)^2 + (bp)^2} \qquad (9)$$

Thus, addition of two integers p and s to parameters of plane layer completely determines the singlewall chiral nanotube structure. By analogy with indexes introduced for carbon nanotubes [10], let's name these integers as chiral indexes of singlewall nanotube (p, s). It is necessary to emphasize that these indexes are expressed in terms of Bravais cells. Taking that into account

$$\sin e_c = \frac{as}{\sqrt{(as)^2 + (bp)^2}} \text{ and } \cos e_c = \frac{bp}{\sqrt{(as)^2 + (bp)^2}}$$

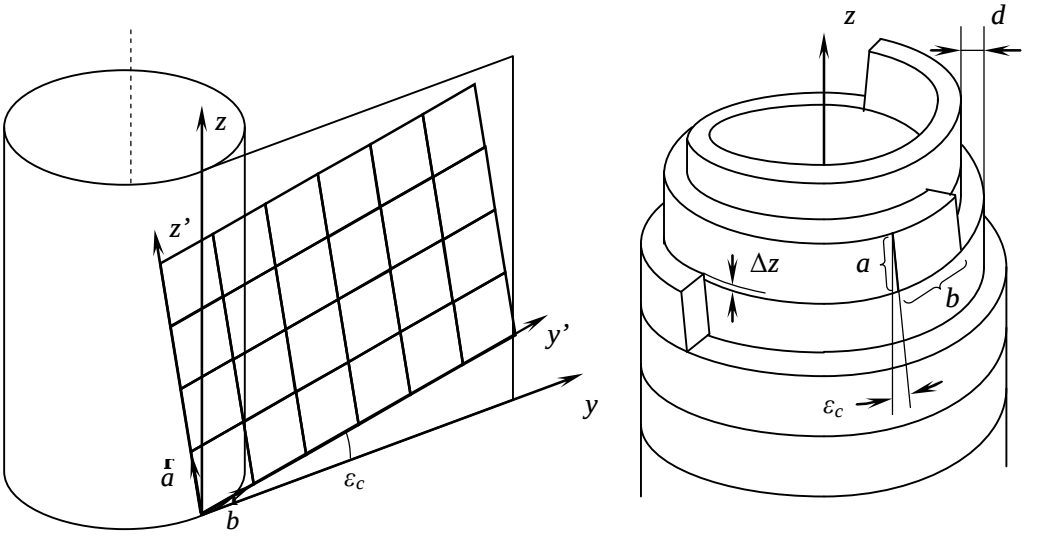
the coordinates of singlewall chiral nanotube atoms can be written down as:

$$\begin{cases} r_j = \dfrac{1}{2p}\sqrt{(as)^2 + (bp)^2} + z_j \\ j_{mj} = 2p\,\dfrac{bp\left(bn + y_j\right) - as\left(an + x_j\right)}{(as)^2 + (bp)^2}. \\ z_{mj} = \dfrac{as\left(bn + y_j\right) + bp\left(an + x_j\right)}{\sqrt{(as)^2 + (bp)^2}} \end{cases} \qquad (10)$$

Let's consider a possibility of existence of multiwall close packed chiral nanotube with radiuses of layers, forming an arithmetic progression. From (1) and (9) it follows that the problem turns into existence of the integer solutions of equation

$$\frac{1}{2p}\sqrt{(as_m)^2 + (bp_m)^2} = r_0 + md \qquad (11)$$

concerning variables p_m and s_m – the chiral indexes of m-th layer. It is obvious that generally there are no such solutions. Hence, multiwall close packed nanotube is possible only if the values p_m and s_m in (11) under condition of (1) become integer owing to small distortions of layer structure. Whittaker pointed this problem in the 50-th of the last century, writing that the layers of a multiwall chiral lattice should have small distortions [4].



a) b)

Fig. 6. The projecting and parameters of the chiral nanotube

There is another possibility that the condition (1) with integers p_m and s_m does not implement exactly. Let's assume that the layers, as it is widely spread among layer crystals, inherit orientation of each other, that is have identical or rather close chiral angles. In this case it is possible to propose the recurrent procedure allowing determination parameters of nanotube layers from parameters of internal layer. Let's assume internal layer has chiral indexes (p_0, s_0), determining its initial radius ρ_0 and chiral angle ε_{c0}. Then the chiral indexes of m-th layer can be determined from ε_{c0} and radius of the previous layer ρ_{m-1} as the nearest integer values of variables

$$p_m = \frac{2p\left(r_{m-1}+d\right)}{b}\cos e_{c0}$$

$$\text{and } s_m = \frac{2p\left(r_{m-1}+d\right)}{a}\sin e_{c0} \qquad (12)$$

and then the chiral angle of layer and its radius – from:

$$\mathrm{tg}e_{cm} = \frac{as_m}{bp_m} \qquad r_m = \frac{1}{2p}\sqrt{\left(as_m\right)^2+\left(bp_m\right)^2}$$

In this model the chiral indexes (p_m, s_m) of all layers are univalently determined by indexes of internal layer (p_0, s_0), therefore the last can be considered as chiral indexes of multiwall nanotube. It is obvious that owing to this procedure the radiuses of multiwall chiral nanotube's layers deviate from progression (1), and their chiral angles ε_{cm} have some variations too (Fig. 7). The proposed procedure of chiral indexes determination can be used both in the nanotubes structural analysis and for calculation of their physical characteristics: band structure, phonon spectrum and so on.

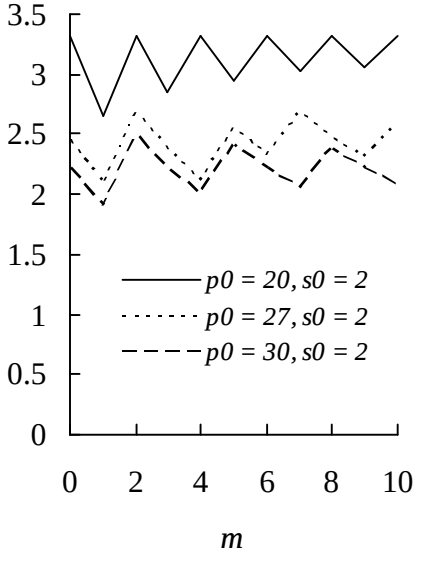


Fig. 7. The dependence of chiral angle ε_{cm} (degrees) on the number of layer

It follows from (12) that, in view of variations associated with rounding off, the number of cells on the turn of helix (first chiral index) can be written down as: $p_m \approx p_0 + mg\cos e_{c0}$.

Hence, if the value $g\cos\varepsilon_{c0}$ – integer, the number of cells on the turn of helix of every layer is integer too (p_0, as well as earlier, is supposed integer), that is a perfect enough chiral nanotube can be formed. The analysis of lattice parameters b and d of plane layer compounds shows that, for example, the generators g of WS_2, MoS_2 and SnS_2 have values 7.11, 7.08 and 5.08, respectively. From experimental data it is known that the chiral type of structure prevails among the corresponding nanotubes and correction to cosine of chiral angle typical value (5–7º) results in much better conformity to integers.

It is possible to write down from (10) the coordinates of multiwall chiral nanotube atoms as:

$$\begin{cases} r_{mj} = \dfrac{1}{2p}\sqrt{\left(as_m\right)^2+\left(bp_m\right)^2}+z_j \\ j_{mmj} = 2p\,\dfrac{bp_m\left(bn+y_j\right)-as_m\left(an+x_j\right)}{\left(as_m\right)^2+\left(bp_m\right)^2}+e_m \\ z_{mmj} = \dfrac{as_m\left(bn+y_j\right)+bp_m\left(an+x_j\right)}{\sqrt{\left(as_m\right)^2+\left(bp_m\right)^2}}+\Delta z_m \end{cases} \qquad (13)$$

parameters ε_m and Δz_m were defined above. The proposed model of multiwall chiral nanotube is not the only possible and complete. The point is that calculations of basal reflexes profiles for some structures at small s_0 shows the presence of superperiod, associated with step character of s_m variation, which is not observed in the experiment. However it seems obvious that at the presence of interlayer splits the system of cylindrical layers can not be strictly coaxial. Thus, it is possible as development of model by displacement of axes of layers up to their contact, and realization of close packing by the linear defects.

4. Roll Nanotube

There is, on the face of it imperceptible, but essential similarity between coaxial and spiral structures: after displacing a coaxial structure layers respectively to each other along the radial cut on thickness of layer d the spiral structure is formed (Fig. 8). This implies that the number of cells on spiral nanotube turn should vary on the value of generator at transition from turn to turn, as in the case of coaxial nanotube at transition from layer to layer.

The crystallographic "directions", corresponding to direction $\vec{b}$ of a roll nanotube layer (Fig. 9), are the three-dimensional spiral-helical lines, which kind depends on

the model of layer. The model of strong layer assumes that it can not have distortions, and the dependence of coordinate *z* of a spiral-helical line's point on the length of its plan projection *L* has linear character: $z = L\mathrm{tg}\varepsilon_c$. Then the chiral angle ε_c is parameter of lattice, but the longitudinal interlayer shift is indefinite. If the layer is capable to distortions (model of elastic layer [7]), the longitudinal interlayer shift can be constant [12] and be used as parameter of lattice. Then dependence $z(L)$ becomes nonlinear and chiral angle becomes indefinite. Let's consider model of strong layer, as available experimental data do not give examples of elastic model.

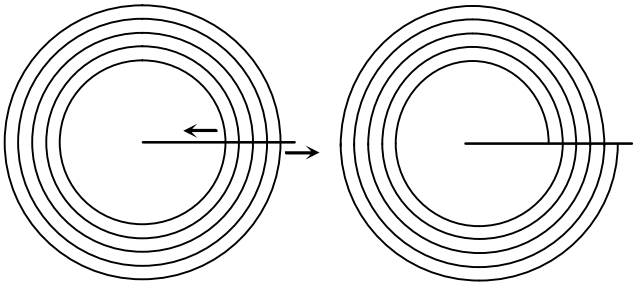


Fig. 8. The mutual transformation of coaxial and spiral structures

An unlimited Archimedes spiral with step *d* looks like:

$$r = t\Phi \qquad t = \frac{d}{2p} \tag{14}$$

where ρ and Φ – polar coordinates.

It follows from (14) that the radiuses of spiral turns form an arithmetic progression that is the spiral structures are close packed by definition. The length of spiral as a function of polar angle:

$$L = t\int_0^{\Phi}\sqrt{1+\Phi^2}\,d\Phi = \frac{t}{2}\left[\Phi\sqrt{1+\Phi^2} + \ln\left(\Phi+\sqrt{1+\Phi^2}\right)\right]$$

In the case of real nanotubes Φ – is large enough value. Hence, it is possible to neglect the unit under radical and the logarithmic addendum, which is the part of a percent from the first. Then:

$$L \approx \frac{t\Phi^2}{2} \tag{15}$$

Let's develop a layer of unlimited roll nanotube on a plane (Fig. 10) keeping orientation (angle ε_c) of its crystallographic directions relative to the nanotube axis. From Fig. 10 it is visible that at constant parameters *a*, *b*, *d*, and ε_c all crystallographic equivalent unlimited roll lattices are determined by displacement the layer lengthways *y'* on a distance $0 \le \Delta b < b$ (is shown in Fig. 10 by shaped line). Any limited (that is having finite internal and external radiuses) roll lattice at the specified constant parameters is a part of one of this unlimited lattices. Parameter Δb, named by azimuthal shift, determines the azimuthal shift polytype modification of roll nanotube.

Thus, the beginning of limited roll lattice is moved along axis *y'* on the distance Δb plus an integer number v_0 of *b*-parameters. Then in the system {*y'*, *z'*} atoms have coordinates: $y'_{nj} = (n_0+n)b + \Delta b + y_j$, $z'_{nj} = an + x_j$ – in a layer's plane and z_j – lengthways the normal. The transformation of coordinates from system {*y'*, *z'*} to system {*y*, *z*} gives:

$$\begin{cases} y_{mj} = \left[(n_0+n)b + \Delta b + y_j\right]\cos e_c - \left(an + x_j\right)\sin e_c \\ z_{mj} = \left[(n_0+n)b + \Delta b + y_j\right]\sin e_c + \left(an + x_j\right)\cos e_c \end{cases}$$

Projecting layer on the roll surface, that is equating y_{nvj} to the value *L* from (15) and taking into account (14), we have:

$$\begin{cases} r_{mj} = \sqrt{2t\left\{\left[(n_0+n)b + \Delta b + y_j\right]\cos e_c - \left(an + x_j\right)\sin e_c\right\}} + z_j \\ \Phi_{mj} = \sqrt{\frac{2}{t}\left\{\left[(n_0+n)b + \Delta b + y_j\right]\cos e_c - \left(an + x_j\right)\sin e_c\right\}} \\ z_{mj} = \left[(n_0+n)b + \Delta b + y_j\right]\sin e_c + \left(an + x_j\right)\cos e_c \end{cases} \tag{16}$$

– the cylindrical coordinates of roll nanotube atoms.

The starting point of a roll lattice corresponds to (16) under condition of equality of values *n*, *v*, x_j, y_j and z_j to zero:

$$\begin{cases} r_0 = \sqrt{2t\,(n_0 b + \Delta b)\cos e_c} \\ \Phi_0 = \dfrac{r_0}{t} = \sqrt{\dfrac{2}{t}(n_0 b + \Delta b)\cos e_c} \\ z_0 = (n_0 b + \Delta b)\sin e_c \end{cases} \tag{17}$$

Let's move the origin of coordinates in this point. Then (16) transforms into:

$$\begin{cases} r_{mj} = \sqrt{r_0^2 + 2t\left[\left(nb + y_j\right)\cos e_c - \left(an + x_j\right)\sin e_c\right]} + z_j \\ j_{mj} = \dfrac{1}{t}\left\{\sqrt{r_0^2 + 2t\left[\left(nb + y_j\right)\cos e_c - \left(an + x_j\right)\sin e_c\right]} - r_0\right\} \\ z_{mj} = \left(nb + y_j\right)\sin e_c + \left(an + x_j\right)\cos e_c \end{cases} \tag{18}$$

– the final expression for coordinates of limited chiral roll nanotube atoms, where $\varphi_{nvj} = \Phi_{nvj} - \Phi_0$.

The term "chiral" is used because here angle ε_c has the same meaning as in case of coaxial chiral nanotubes - orientation of one of the layer's crystallographic directions relative to the nanotube axis. Unlike the coaxial chiral nanotubes, in this case a chiral angle ε_c determines simultaneously both rotary and longitudinal shift (monoclinic) polytype modifications, as it sets both the turn of layer relative to direction of nanotube's axis and the interlayer shift. In case $\Delta b = 0$ and $\varepsilon_c = 0$ the polytype modification is called orthogonal.

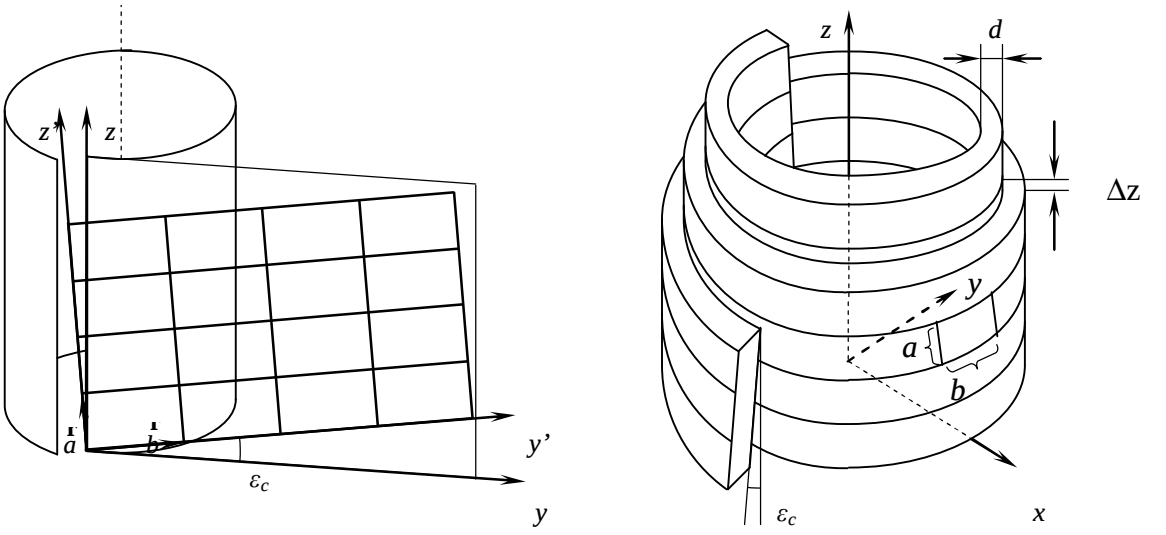


Fig. 9. The projecting and parameters of the roll nanotube

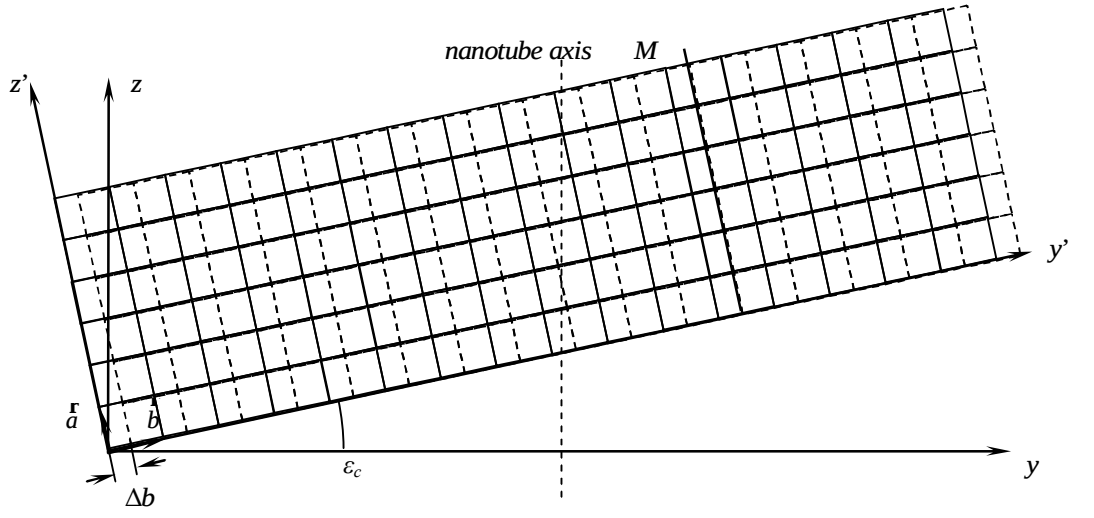


Fig. 10. The roll layer developed on a plane

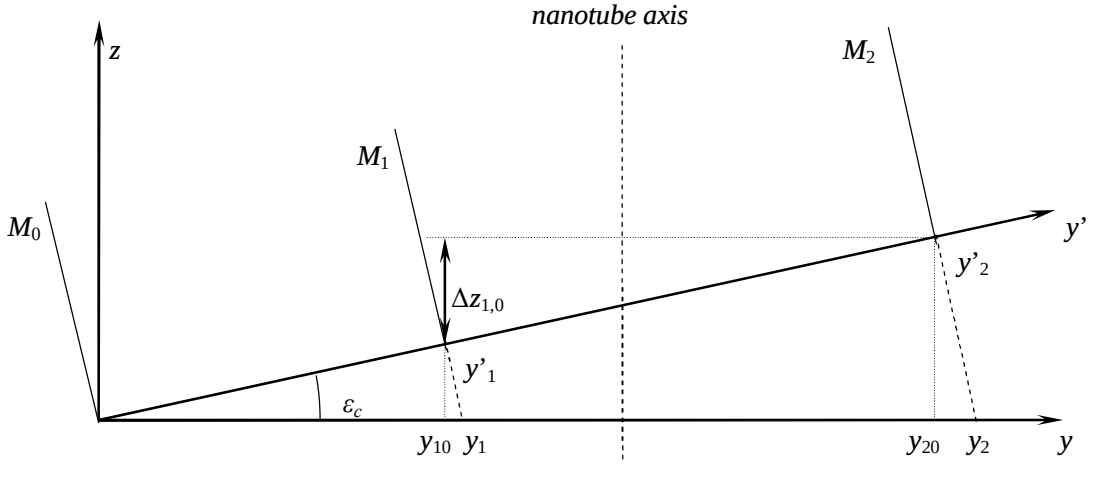


Fig. 11. The spiral-helical line developed on a plane

Let's divide a roll lattice into the turns. In Fig. 11 the limited three-dimensional spiral-helical line *y'*, developed on a plane {*y*, *z*}, is shown, M_m – initial lines of roll nanotube turns (as *m*-th is named the turn, the starting radius of which corresponds to this value of *m*). The length ΔL of the limited plan spiral, according to (15) and (17) looks like:

$$\Delta L = L - L_0 = \frac{t}{2}\left(\Phi^2 - \Phi_0^2\right) = \frac{tj}{2}\left(\frac{2r_0}{t} + j\right) = r_0 j + \frac{tj^2}{2} \quad (19)$$

at $\varphi = 2\pi m$ it is possible to obtain coordinates of crossing points of *y*- and *y'*-axes with *m*-th turn's initial line:

$$y_m = \Delta L_m = 2p r_0 m + p\,dm^2$$

$$y'_m = y_m \cos e_c = \left(2p r_0 m + p\,dm^2\right)\cos e_c \quad (20)$$

Hence (Fig. 11), *y*-coordinate of starting point of the *m*-th turn

$$y_{m0} = y'_m \cos e_c = \left(2p r_0 m + p\,dm^2\right)\cos^2 e_c$$

Equating this to expression (19) we obtain the azimuthal

$$j_{m0} = \frac{1}{t}\left(\sqrt{r_0^2 + 2t\,y_{m0}} - r_0\right) \quad (21)$$

and from (20) –

$$z_{m0} = y'_m \sin e_c = \left(2p r_0 m + p\,dm^2\right)\sin e_c \cos e_c \quad (22)$$

longitudinal coordinates of starting points of the spiral's turns, and also the longitudinal interlayer shift in these points

$$\Delta z_{m0} = z_{m+1,0} - z_{m0} = \left[2p r_0 + p\,d\,(2m+1)\right]\sin e_c \cos e_c \quad (23)$$

It is necessary to notice, the less is relation d/ρ_0, the less is longitudinal interlayer shift dependence on the layer number *m*.

Let's calculate the length of the *m*-th turn. From (20):

$$\Delta y'_m = y'_{m+1} - y'_m = \left[2p r_0 + p\,d\,(2m+1)\right]\cos e_c$$

Then the number of parameters *b*, going in the *m*-th turn,

$$p_m = \frac{\Delta y'_m}{b} = \left(\frac{2p r_0}{b} + \frac{2p\,d}{b}m + \frac{p\,d}{b}\right)\cos e_c =$$

$$= \left(\frac{2p r_0}{b} + mg + \frac{g}{2}\right)\cos e_c \quad (24)$$

The generator *g*, previously introduced, appears in the right part of (24). In a practically important case of small ε_c (24) transforms in:

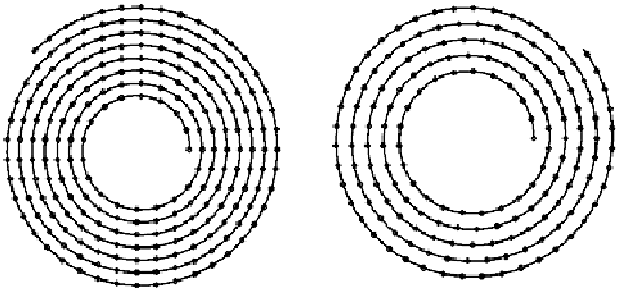
$$p_m \approx \frac{2p r_0}{b} + mg + \frac{g}{2} = p_0 + mg + \frac{g}{2},\ p_0 = \frac{2p r_0}{b}$$

that is at transition from turn to turn the number of sites on a turn changes on the value of generator as for circular lattices. If p_0 is integer the numbers p_m are integers or semi-integers depending on the evenness or oddness of the generator, accordingly. Hence, in such roll lattices with even generator each turn starts from site; in the case of odd generator the even turns starts from site, but odd ones – from interstitial. In particular, the unlimited and so-called "multiple" lattices, in which initial radius ρ_0 is equal to an integer number of parameters *d*, are the same (Fig. 12).

In the case of small ε_c expressions (21)-(23) transform into $j_{m0} = 2p\,m$, $z_{m0} \approx \left(2p r_0 m + p\,dm^2\right)e_c$, $\Delta z_{m0} \approx \left[2p r_0 + p\,d\,(2m+1)\right]e_c$, respectively, and the initial radiuses of turns correspond to (1). Each turn of the multiple structure with even generator, and also an even turn of the structure with odd generator start from the site, therefore coordinates of their atoms can be determined from (18) in approach of small ε_c by replacement $\rho_0 \to \rho_m$ and addition of the value z_{m0} from (22) to *z*-coordinate. The azimuthal angle of atom φ_{mnvj} thus measured from the beginning of appropriate turn is:

$$\begin{cases} r_{mnvj} \approx \sqrt{r_m^2 + 2t\left[nb + y_j - \left(an + x_j\right)e_c\right]} + z_j \\ j_{mnvj} \approx \dfrac{1}{t}\left\{\sqrt{r_m^2 + 2t\left[nb + y_j - \left(an + x_j\right)e_c\right]} - r_m\right\} \\ z_{mnvj} = an + \left(2p r_0 m + p\,dm^2 + nb + y_j\right)e_c + x_j \end{cases} \quad (25)$$

In the case of even generator index $n = 0$-$(p_m$-$1)$. There are p_m-1/2 whole unit cells or p_m+1/2 sites belonging to this turn in the case of even turns of structure with odd generator. Hence, index *v* vary in limits $n = 0$-$(p_m$-$1/2)$.



a) b)

Fig. 12. The cross-sections of the multiple roll lattices with $g = 4$ (a) and $g = 5$ (b)

In the case of odd turns of structure with odd generator each turn starts from interstitial, which means addition of value 1/2 to the index *v* in (25):

$$\begin{cases} r_{mnvj} \approx \sqrt{r_m^2 + 2t\left[(n+1/2)b + y_j - \left(an + x_j\right)e_c\right]} + z_j \\ j_{mnvj} \approx \dfrac{1}{t}\left\{\sqrt{r_m^2 + 2t\left[(n+1/2)b + y_j - \left(an + x_j\right)e_c\right]} - r_m\right\}. \\ z_{mnvj} = an + \left[2p r_0 m + p\,dm^2 + (n+1/2)b + y_j\right]e_c + x_j \end{cases}$$

Here the p_m-1/2 of whole unit cells take place too. However the number of sites belonging to this turn is equal to p_m-1/2 too, as the "last" site of odd turn does not belong to it, but is the "first" for the following (even) turn. This means that index n vary in limits n = 0-(p_m-3/2) on the odd turn. The case of the odd generator and semi-integer $p_0 = 2\pi\rho_0/b$ is the very same as the case of even generator.

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КРИСТАЛОГРАФІЯ КОАКСІАЛЬНИХ І СПІРАЛЬНИХ НАНОТРУБОК ДОВІЛЬНОГО СКЛАДУ

Анотація. *Отримано циліндричні координати атомів багатошарових ахіральних, хіральних та спіральних нанотрубок довільного хімічного складу внаслідок проектування структури плоского аналогу на відповідну поверхню. Для опису структури нанотрубок використано коаксіальні та спіральні циліндричні решітки, комірки Браве та індекси хіральності, виражені в цих комірках. Запропоновано модель багатошарової хіральної нанотрубки з нещільним пакуванням шарів.*

Ключові слова: *нанотрубка, хіральний, спіральний, рулон.*