Computation of full symmetry group of C_4C_8(R) nanotubes using a mathematical model

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The full symmetry group of C_4C_8(R) nanotubes are investigated. We introduce the nanotube graphs as metric spaces and consider their isometries to compute their symmetry groups. It is shown that the symmetry group of a chiral nanotube with chiral vector c, is isomorphic to Gc =< x, y, z | $x^n = z^2 = (zx)^2 = (yz)^2 = 1$, xy = yx, o(y) = ∞ >.

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1. Introduction

Carbon nanotubes, which are multi-walled structures of pure carbon, were discovered in 1991 [1]. They show remarkable mechanical properties and extensive experimental and theoretical investigations have been carried out on them [2–4]. Their mechanical characteristics clearly predestinate them for advanced composites. A single-wall carbon nanotube is a cylindrical structure with a diameter of a few nanometres; it is periodic along its axis and can be visualized as a rolled-up honeycomb lattice. Nanotubes are attractive subjects for study in solid-state physics due to their potential applications in nanotechnology. Their symmetry is important in theoretical investigations and has been investigated (see [5]-[10]). The high symmetry of carbon nanotubes has facilitated the theoretical investigation of the physical phenomena occurring in these materials.

A C_4C_8 net is a trivalent decoration made by alternating squares C4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation [11]. Optimized C_4C_8 net covering a nanotube is illustrated in Figure 2. Such nanotubes could appear by successive low energy Stone- Wales [12] edge flipping in polyhex nanotubes [11].

Because the relation between the carbon atoms and the symmetry operations is one-to-one, the nanotubes can be viewed as a realization of the line groups. In order to find the symmetry groups of carbon nanotubes, the symmetry operations of grapheme are considered. Those that are preserved when the graphene sheet is rolled into a cylinder form the nanotube symmetry group.

The full symmetry group of square C_4C_8 nanotubes, C_4C_8(S), were computed in [13] by introducing a mathematical model. In this paper we consider the rhomb C_4C_8 nanotubes, C_4C_8(R), and we compute their full symmetry groups.

2. Main results and discussion

The cylindrical portions of the tubules consist of a single C_4C_8(R) lattice that is shaped to form the cylinder. It is convenient to specify a general C_4C_8(R) nanotube in terms of the tubule diameter d, and the chiral angle θ. The unit cell is spanned by two basis vectors a_1 and a_2 with same length $a_1 = a_2 = a_0$ which form an angle of $\pi/2$. In C_4C_8(R) nanotubes, the lattice is rolled up in such a way that a lattice vector $c = n_1a_1+n_2a_2$ becomes the circumference of the tube. This circumferential vector c, which is denoted by (n_1, n_2), is called chiral vector and uniquely defines a particular tube.

Now we present the lattice C_4C_8(R) nanotube as a metric space. Let us consider the vectors

$$e_1 = (1,0), e_2 = (-\sqrt{2}/2, -\sqrt{2}/2),$$
$$e_3 = (-\sqrt{2}/2, \sqrt{2}/2), e_4 = (0,1).$$

Put $a_1 = e_1-e_2-e_3$ and $a_2 = e_2-e_3-e_4$ as shown in Fig. 1.

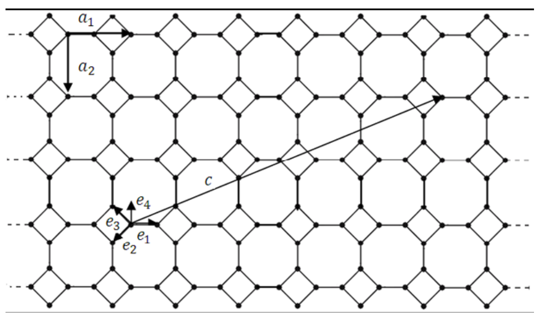

Fig. 1. Two dimensional lattice of C_4C_8(R) Nanotube.

The periodic set, $\Gamma = \{n_1a_1 + n_2a_2 \mid (n_1, n_2) \in L\}$ where $L = L^0 \cup L^1 \cup L^2 \cup L^3$,

$$L^0 = Z^2, L^1 = L^0 + (\sqrt{2}/(2+\sqrt{2}), 0),$$
$$L^2 = L^0 + (-1/(2+\sqrt{2}), 1/(2+\sqrt{2})),$$
$$L^3 = L^0 + (-1/(2+\sqrt{2}), -1/(2+\sqrt{2}))$$

is the C_4C_8(R) lattice. Instead of the basis $\{a_1,a_2\}$, we have the possibility to use vectors e_1,e_2,e_3 and e_4.

Theorem 1. There is a bijection $\psi:\ell\to\Gamma$,

$\psi(x)=x_1e_1+x_2e_2+x_3e_3+x_4e_4$. from the set

$$\ell = \{(x_1,x_2,x_3,x_4)\in Z^4 \mid x_1+x_2+x_4\in\{0,1\},\ x_1+x_3-x_4\in\{0,1\}\}$$

to the set Γ of all vertices of C_4C_8(R) lattice.

Proof. It is clear that ψ is well-defined. We show that this map is 1-1 and onto. Let $\psi(x)=\psi(y)$. By considering the vectors e_i, we have we $y_1-\sqrt{2}(y_2+y_3)/2 = y_1-\sqrt{2}(y_2+y_3)/2$ and $-\sqrt{2}(x_2-x_3)/2+x_4 = -\sqrt{2}(y_2-y_3)/2+y_4$. So

$$x_1-y_1=\sqrt{2}(x_2+x_3-(y_2+y_3))/2\ ,$$
$$x_4-y_4=\sqrt{2}(x_2-x_3-(y_2-y_3))/2\,.$$

But the coordinates of x and y are integers, therefore $x_1=y_1$, $x_4=y_4$, $x_2+x_3=y_2+y_3$ and $x_2-x_3=y_2-y_3$. Consequently we have x=y. Therefore ψ is 1-1.

Now let $v\in V(T)$. Without loss of generality, let $v\in L^2$. Since we have $\psi(n,m-n+1,-m-n,-m)=v$ and it is easy to check that $(n,m-n+1,-m-n,-m)$ is an element of ℓ. The subset ℓ of Z^4 becomes in this way a mathematical model for the vertex set of C_4C_8(R) nanotubes. It is easy to check that $\ell=\bigcup_{i=1}^4 T_i$ where

$$T_1=\{(x_1,x_2,x_3,x_4)\in\ell \mid x_1+x_2+x_4=0, x_1+x_3-x_4=0\},$$
$$T_2=\{(x_1,x_2,x_3,x_4)\in\ell \mid x_1+x_2+x_4=0, x_1+x_3-x_4=1\},$$
$$T_3=\{(x_1,x_2,x_3,x_4)\in\ell \mid x_1+x_2+x_4=1, x_1+x_3-x_4=0\},$$
$$T_4=\{(x_1,x_2,x_3,x_4)\in\ell \mid x_1+x_2+x_4=1, x_1+x_3-x_4=1\}.$$

The mapping d: $\ell\times\ell \to N$ where $d(x,y)=\sum_{i=1}^4 |x_i-y_i|$ is the L_1-norm and so is a distance function on ℓ, moreover x is a k-neighbor of y if d(x, y) = k.

The nearest neighbors of $x=(x_1,x_2,x_3,x_4)$ are

$x^1=x+\varepsilon_1(x)f_1+\varepsilon_4(x)f_4$, $x^2=x+\varepsilon_2(x)f_2$, and $x^3=x+\varepsilon_3(x)f_3$

where $\varepsilon_2(x)=(-1)^{x_1+x_2+x_4}$, $\varepsilon_3(x)=(-1)^{x_1+x_3-x_4}$,

$$\varepsilon_1(x)=\varepsilon_3(x)\chi_{T_1\cup T_4}(x), \varepsilon_4(x)=\varepsilon_3(x)\chi_{T_2\cup T_3}(x)$$

$f_1=(1,0,0,0)$, $f_2=(0,1,0,0)$, $f_3=(0,0,1,0)$, $f_4=(0,0,0,1)$ and χ_A is the characteristic function on the set A which has value 1 on A and 0 outside of A.

The graph $\zeta=(\ell,\xi)$, where $\xi=\{\{x,y\}\mid x,y\in\ell, d(x,y)=1\}=\{\{x,x^i\}\mid x\in\ell, i\in\{1,2,3\}\}$ can be associated to the metric space (ℓ, d) in a natural way where x^1,x^2,x^3 are the nearest neighbours of x.

An isometry of the metric space (M, d) is a bijection $f : M \to M$ such that $d(x, y) = d(f(x), f(y))$, for all $x, y\in M$. It is easy to see that the composition of two isometries is again an isometry and so the set of all isometries of a metric space is a group with the composition of isometries. A graph-automorphism of graph G is a bijection that preserve the edges. Any isometry is a graph-automorphism.

Lemma 1. Transformations σ, τ, $\rho_a:\ell\to\ell$, where

$$\sigma(x)=(-x_1,-x_3+1,-x_2+1,x_4)$$
$$\tau(x)=(x_4,x_2,-x_3+1,x_1)$$
$$\rho_a(x)=\begin{cases} x+a & a\in T_1\\ x+a+(0,0,-1,0) & a\in T_2\\ x+a+(0,-1,0,0) & a\in T_3\\ -x+a & a\in T_4\end{cases}$$

where $x=(x_1,x_2,x_3,x_4)$, are isometries of the metric space (ℓ,d) for any $a\in\ell$.

Proof. It is easy to check that σ, τ, ρ_a are well-defined bijections and preserve the distance.

Now we are ready to give the symmetry group of C_4C_8(R) lattice using the isometries of metric space (ℓ, d).

Theorem 2. Let G be the symmetry group of the C_4C_8(R) lattice. Then

$G =< \sigma, \tau, \rho \mid \sigma^2 = \tau^2 = \rho^2 = (\rho\tau\sigma\tau)^2 = (\sigma\tau)^4 = 1, \rho\sigma \neq \sigma\rho, \rho\tau\neq\tau\rho >$ where $\rho = \rho_{(1,0,0,0)}$, σ and τ are as defined in Lemma 1.

Proof. The group G coincides with the group of all the isometries of the metric space (ℓ, d). The transformations σ, τ and ρ are isometries of the metric space (ℓ, d). The origin point O = (0, 0, 0, 0) can be transformed into an arbitrary point of ℓ by composing these transformations. It is easy to check that $\sigma\tau$, τ, $\rho\tau$ are corresponding to the fourfold rotation, vertical mirror plane, and (I|01). The relations between generators of group can be easily obtained.

Let H be the subgroup of translations. Then

$$H =< a, b \mid ab = ba, o(a) = o(b) = \infty > \cong = Z\oplus Z$$

where $a = \rho_{(1,-1,-1,0)}$ and $b = \rho_{(0,1,-1,-1)}$.

Now we describe the C4C8(R) nanotubes using our model as follows.

An C_4C_8(R) nanotube can be visualized as the structure obtained by rolling a C_4C_8(R) lattice such that the endpoints of a translation vector c are folded one onto the other (see Fig. 1). The vector c is the chirality of the tubule. In our model, an C_4C_8(R) nanotube is described by the element c = (c1, c2, c3, c4) of translations. Let c be a fixed translation. The relation $x \sim y \leftrightarrow x - y \in Zc$ is an equivalence relation on ℓ. The equivalence class corresponding to $x\in\ell$ is $[x] = x + Zc = \{x + kc \mid k \in Z\}$.

It is easy to check that $\varepsilon_1(c) = \varepsilon_2(c) = \varepsilon_3(c) = 1$, $\varepsilon_4(c) = 0$, and for any $x \in \ell$ we have $\varepsilon_i(x + kc) = \varepsilon_i(x)$ for i = 1, 2, 3, 4 and $k \in Z$. Thus if $y \in [x]$ then $y^i \in [x^i]$ for i = 1, 2, 3. If we define $[x]^i = [x^i]$ and consider the graph $\zeta_c = (\ell_c, \xi_c)$, where

$$\ell_c = \{[x] \in Z^4/Zc \mid x \in \ell\}$$
$$\xi_c = \{\{[x], [x]^i\} \mid [x] \in \ell_c\}$$

the set ℓ_c can be used as a mathematical model for an $C_4C_8(R)$ nanotube with chiral vector c.

A symmetry transformation of the $C_4C_8(R)$ lattice $g : \ell \to \ell$ defines the symmetry transformation $g_c : \ell_c \to \ell_c$, where $g_c([x]) = [g(x)]$ of the $C_4C_8(R)$ nanotube ℓ_c if $[x] = [y]$ then $[g(x)] = [g(y)]$, for every $x, y \in \ell$.

Theorem 3. For any $w \in \ell$, the transformation $g_w : \ell_c \to \ell_c$;$g_w[x] = [\rho_w(x)]$ is a graph-automorphism of ℓ_c.

Proof. Let [x] = [y]. Since $x - y \in Zc$ if and only if $\rho_w(x) - \rho_w(y) \in Zc$ the transformation g_w is well-defined and preserves the adjacency.

On can remark that $g_w([x]^i) = (g_w[x])^i$ for all $x \in \ell$ and $i \in \{1, 2, 3\}$.

Now we are ready to compute the full symmetry group of $C_4C_8(R)$ nanotubes using our model.

Let $n = \gcd\{c_1, c_2, c_3, c_4\}$ and $c' = c/n$. The transformation $g_{c'}$ represents a rotation of angle $2\pi/n$ of the nanotube with respect to its axis. Since $(c_2-c_3-c_4)c_1+(-c_1+2c_3+c_4)c_2+(c_1-2c_2+c_4)c_3 +(c_1-c_2-c_3)c_4 = 0$, the vector $a = (c_2-c_3-c_4,-c_1+2c_3+c_4, c_1-2c_2+c_4, c_1-c_2-c_3)$ is orthogonal to c, and the corresponding transformation ga is a pure translation, that is, a translation in the direction of the nanotube symmetry axis. The vector t =a/N where $N = \gcd\{c_2-c_3-c_4,-c_1+2c_3+c_4, c_1-2c_2+c_4, c_1-c_2- c_3\}= 3\gcd\{-c_4, c_3,-c_2, c_1\} = 3n$, defines the shortest pure translation of ℓ_c.

Let $x=(x_1,x_2,x_3,x_4) \in T_1$ and $y=(y_1,y_2,y_3,y_4) \in T_1$. Then one can see that $< x, y >= (3+2\sqrt{2})(x_1y_1 +x_4y_4)$ where $< x, y >$ is the usual scalar product of x and y.

It is easy to check that $||t||=||c||/n$ where $||c||^2= 3c_1^2 +\sqrt{2}c_2^2+\sqrt{2}c_3^2+3c_4^2$. Hence the number q of lattice units in the nanotube unit cell is $q = (c_1^2++c_4^2)/n$.

For any $x=(x_1, x_2, x_3, x_4) \in T_1$, the projections of x in c and t directions can be written as

$$<x,c>c/||c||^2=(x_1c_1/n+x_4c_4/n)c/q \in Zc/q,$$
$$<x,t>t/||t||^2=(-x_1c_4+x_4c_1)t/q' \in Zt/q',$$

where $q' = q/n$.

Theorem 4. Let G_c be the symmetry group of chiral infinite $C_4C_8(R)$ nanotube, $x = g_{c'}$, $y = g_w$ and $z = g_{(1,0,0,0)}$ where $w \in T_1$ is the shortest vector such that $<w,t>t/||t||^2=t/q'$. Then we have

$$G_c =< x, y, z \mid x^n = z^2 = (zx)^2 = (yz)^2 = 1, xy = yx, o(y) = \infty > .$$

Proof. From the geometry of $C_4C_8(R)$ nanotubes and previous explanations, the generators of the symmetry group are true. One can easily justify the relations between generators.

3. Conclusion

In this work a mathematical model for $C_4C_8(R)$ nanotubes is given. The lattice of the nanotube is introduced as a metric space. Using this metric space, we computed the full symmetry group of the nanotube. Our model is very useful for computing the distance-based invariants of the graph of nanotube.

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