Diamane Fibonacci Nanotubules for Quantum Computing

Hans Hermann Otto

Formerly Materials Science and Crystallography, Clausthal University of Technology, Clausthal-Zellerfeld, Lower Saxony, Germany

E-mail: hhermann.otto@web.de

Abstract

We propose 13-protofilament *Fibonacci* nanotubules of diamane for quantum computing. Generated color centers acting as qubits may have coherence times greater than a minute and a processing temperature much higher than 1 K enabling the construction of energy-efficient computers. The proposal paws the way to develop purely organic hollow nano-fibers for quantum computing operating around room temperature, where qubits are better protected against noise decoherence. However, 2*D* diamond structures are superior with regard to thermal stability and will therefore retain lasting importance in computational and sensor technology.

Keywords: Quantum Computing, 2D-Diamonds, Diamenes, Fibonacci Nets, 13-Protofilament Nanotubules.

Perspective for New Quantum Computer Chip Material

Diamond-based technology will be the dominant for the next decade of quantum computing. We have learnt to generate color centers in diamond acting as qubits that are able to process information with controllable bit coherence times over a minute at temperature of greater than 1K [1] [2] [3]. Point defects such as NV or SiV centers in diamond can be atomically precise manufactured by recoil implantation, where a gallium focused-ion-beam is exposed to a thin layer of silicon nitride on a diamond surface [4]. However, the thin layer material diamane consisting of sp^3- hybridized carbon atoms can be synthesized by intense pressure acting on a two-layer graphene sheet (graphene diamondization). The material indicated high thermal conductivity, high thermal stability, high oxidation resistance, and has a large band gap [1]. Certainly it can be up-rolled to a nanotubule [5]. Most interesting would be a hollow tubule with a protofilament number of 13, copying nature's favorite and successful microtubule strategy [5] [6]. We can start the synthesis with double-walled carbon nanotubes (DWCNT's), where one tube settles inside the other. The most favorable position of the two tubes relative to each other must be found in order to keep the atomic mismatch as small as possible. Then we apply pressure on the tubes to transform the sp^2-bonded material into sp^3-bonded diamane. Stability against bursting could be achieved by filling the hollow tube with, for instance, liquid gallium that have no tendency to react with carbon atoms and is used as catalytic mediator for the diamond synthesis [7]. The soliton character of nanotube diamene would

guarantee progress in both qubit coherence time and processing temperature. The need of outsourcing quantum computing in the orbit in order to cool the computers cost efficiently may become superfluous, if the processing temperature is enhanced towards room temperature. As a realistic perspective, the successful production of the proposed material opens the way for a further development towards purely organic nanotubules for information processing operating near room temperature through dissipation-free energy tranfer, a dream for the mankind. However, 2*D* diamond structures are superior with regard to thermal stability and will therefore retain lasting importance in computational and sensor technology.

The reader may better understand the synthesis proposal by looking at the pictures of planar *Fibonacci* nets given in reference [5]. The construction of a chiral graphene net composed of 13 hexagons is explained, which can be rolled up to a nanotubule (**Figure 3**).

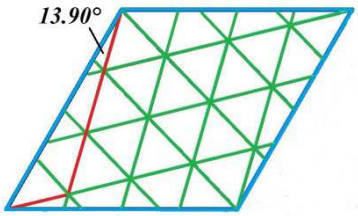

Figure 1. Fibonacci arrangement of a hexagonal net consisting of 13 subcells, offset by an angle of 13.9° in comparison to the blue outlined ‘unit cell’.

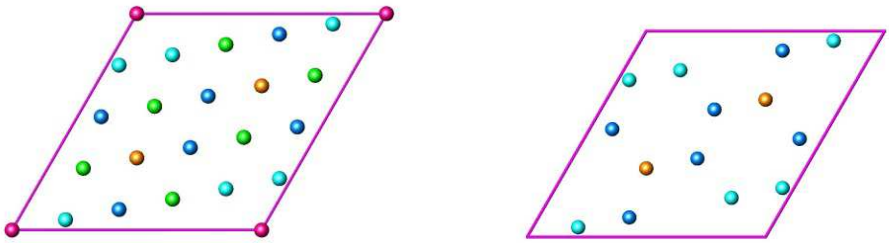

Figure 2. *Fibonacci* cell with 21 atoms (left) respectively downsized to 14 atoms (right). Symmetry equivalent positions have given a common color.

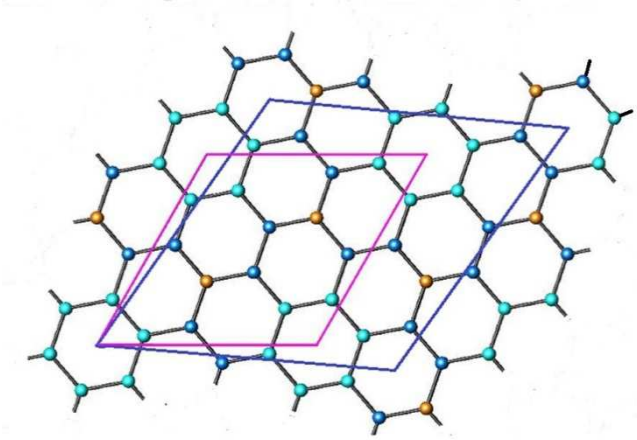

Figure 3. Chiral graphene net composed of 13 hexagons within the blue outlined ‘unit-cell’.

Distances between inner and outer carbon cylinders are governed by *van der Waals* interactions, which are actually *Casimir-Lifshitz* forces [8]. The distances range from 3.4 Å to 3.8 Å with extreme limits of 2.86 respectively 4.2 Å, depending on the chirality.
Rolling up a *Fibonacci* carbon net to a nanotubule would deliver a diameter *D* of about 10(Å) based on the C-C distance within the graphene sheet of $a_{cc} = 1.42$ (Å) (see formula (16)). This diameter yields for the inner tubule. The outer tubule diameter would have a value of about 16.7 (Å). The chirality is given by the offset angle α_F between sub-cell direction and *a*-axis of the graphene net. The angle is only changed insignificantly when the net is rolled up

$$\alpha_F = arctan\left(\frac{5}{3\sqrt{3}}\right) - 30 = 13.898° \approx \frac{180}{13}. \tag{1}$$

This angle is very remarkable through its relation to *Sommerfeld*'s reciprocal fundamental constant α^{-1} [9] 10] [11]

$$\alpha^{-1} \approx \alpha_F \cdot \pi^2 \tag{2}$$

It is one of the big secrets surrounding microtubules with protofilament number 13. Another relation connects α_F with *Guynn*'s galactic velocity β [10] [12] respectively with the circle constant π or the golden mean $\varphi = \frac{\sqrt{5}-1}{2} = 0.6180339887$ ...

$$\beta \approx (\pi^4 \alpha_F)^{-1} \tag{3}$$

$$\alpha_F \approx 4\pi + \frac{\pi+1}{\pi} = 13.88468 \tag{4}$$

$$\alpha_F \approx \frac{1}{\pi^2}\left(360\varphi^2 - 2\varphi^3 + \left(\frac{\varphi}{3}\right)^5\right) = 13.88465 \tag{5}$$

Equation (5) used the depiction of α^{-1}in terms of the golden mean given by *Pellis* [13] [14]. The frequent connection of α_F with fundamental respectively universal numbers expresses geometrical entanglement as a prerequisite for quantum entanglement.

Chirality correlation in double-wall carbon nanostructures were studied in detail by *Hirahama et al.* [15]. The *DWNT*'s were synthesized by the arc discharge method. The authors provided a formula for the chiral angle that we denote by δ

$$\tan(\delta) = \frac{\sqrt{3}\cdot m}{2n+m} \tag{6}$$

where (*n*,*m*) represents the chiral index. For *m* = 1 and *n* = 3 we obtain the chiral angle

$$\delta = \alpha_F = 13.89788° \tag{7}$$

However, the formula (6) was already given by the present author in a similar form by using the *Miller* indices h and k between graphene-cell direction and big unit-cell direction (**Figure 1**) [5] [6] [10] [11] [16]

$$\delta(°) = \arctan\left(\frac{h+2k}{h} \cdot \frac{1}{\sqrt{3}}\right) - 30 = \arctan\left(\frac{k}{2h+k} \cdot \sqrt{3}\right) \tag{8}$$

So we don't need the indices m and n and should use the more familiar *Miller* indices h and k in order to characterize chirality.
Unfortunately, the formula for the diameter D of the chiral nanotubules given in reference [15] is wrong. If you ask *AI* for the carbon tubular diameter formula, you get the wrong one. Therefore we will present approximated and exact formulas and check whether *AI* is capable of learning.
Chirality of a twisted hexagonal carbon net is represented by the index sum of squared *Miller* indices

$$\Sigma = h^2 + k^2 + hk \tag{9}$$

A helix of length l_0 and height z_0 is projected down the z axis to give a circle of diameter D. Applying the *Pythagorean* theorem we get

$$l_0^2 = z_0^2 + \pi^2 D^2 \tag{10}$$

The height of a helical single turn is

$$z_0 = a_{cc}\sqrt{3} \cdot \sqrt{\Sigma} \tag{11}$$

and the length can be approximated by

$$l_0 \approx a_{cc}\sqrt{3} \cdot \Sigma \tag{12}$$

where a_{cc} is the carbon-carbon spacing.

Then we obtain for the diameter

$$D \approx \frac{a_{cc}\sqrt{3}}{\pi} \cdot \sqrt{\Sigma^2 - \Sigma} \tag{13}$$

A better approximated formula is given by

$$D \approx \frac{a_{cc}\sqrt{3}}{\pi} \cdot \Sigma \cdot \cos(\delta) \tag{14}$$

The exact formula is

$$D = \frac{a_{cc}\sqrt{3} \cdot \cos(\delta)}{\sin(\frac{180}{\Sigma})} \tag{15}$$

For a 13-protofilament helix we obtain according to formula (13) to formula (15)

$D \approx 9.78(\text{Å})$ formula (13)
$D \approx 9.88(\text{Å})$ formula (14)
$D = 9.98(\text{Å})$ formula (15)

There exists only two *Fibonacci* helices in the low indices range, characterized by $\Sigma = 13$ and $\Sigma = 21$. The diameter for the 21-protofilament tubule is calculated to be about 16.2(Å) and would match the 16.7(Å) distance requirement for the outer tubule (see **Table 1**). A double-walled carbon nanotube consisting of the two *Fibonacci* tubules is a very interesting case, even if their compression to a diamane tubule may be an elaborated task.

Table 1. Geometry of Planar Hexagonal Nets and Rolled-up Tubules

The 'lattice parameter' $\boldsymbol{a = a_{cc} \cdot \sqrt{3} \cdot \sqrt{\Sigma}}$ representing the repetition length of the tubules was calculated using the carbon distance within graphene, $a_{cc} = 1.42(\text{Å})$ (see **Figure 3**). Miller indices *h* and *k*, *D* = diameter of the tubules, δ = angle of chirality

$\boldsymbol{h}$	$\boldsymbol{k}$	$\boldsymbol{\Sigma = h^2 + k^2 + h \cdot k}$	$\boldsymbol{a}$	$\boldsymbol{\delta}(°)$	D
1	1	3	4.260	30	2.459
2	1	7	6.507	19.1066	5.356
2	2	12	8.520	30	8.229
3	1	**13**	8.868	**13.8979**	**9.976**
3	2	19	10.721	23.4132	13.712
4	1	**21**	11.271	**10.8934**	**16.205**
3	3	27	12.780	30	18.347
5	1	31	13.694	8.9482	24.015

The case with $\boldsymbol{\Sigma = 3}$ is not realistic. An example is lead germanate $PbGe_4O_9$, where germanate dreier rings (α -phase) are broken to give flat screwed chains (γ-phase) [17] [18]. Germanate are interesting, because ß-$PbGeO_3$ shows an extreme layer structure like graphene [19].

The wanted chiral carbon tubules can be synthesized by high-power laser ablation of a graphite target supported by mixed metallic catalysts such as Ni, Co and in addition Ga and condensation onto a graphene tubule substrate of specified chirality at moderately high temperatures. Also the direct diamene tubule synthesis can be figured out, when once a first diamene tubule substrate is available. Then NV color centers could directly generated by applying an argon protecting gas with some nitrogen added. High electric conductivity and high stability of diamene tubules can be assumed.
The explained geometry of hexagonal nets is applicable also to layered double hydroxides [16].
Finally, we recommend studying the contribution of *Zhang* and coworkers [20] about the use of spin arrays on *DNA* in combination with NV centers in diamond for quantum technological applications as an example for combined structures that can hopefully soon be replaced by diamane tubule based technology.

Conclusion

The synthesis of double-wall carbon nanotubules consisting of helices with protofilament *Fibonacci* number 13 (inside) and 21 (outside) is suggested and their catalysis-assisted transformation into diamane tubules by pressure. Another synthesis route is laser ablation. The use of gallium as catalytic mediator is emphasized. *NV* color centers in this helical 2*D* diamond material could act as qubits rendering it as new stable material of high electric conductivity for energy-efficient quantum computers. Helical inorganic materials may serve as examples for future organic quantum computer materials finally operating at room temperature. It suggests what nature always uses.

Conflicts of Interest

The author declares no conflict of interests regarding the publication of this paper. No artificial intelligence was used.

The author apologizes for some typographical errors in previous drafts.

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