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The Architecture of Sierpinski Knots

Jin-Wei Duan, Zhen Zheng, Pan-Pan Zhou, Wen-Yuan Qiu[1]

Department of Chemistry, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

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Abstract: To understand the growth and transformation mechanisms of DNA fractal knots, a series of Sierpinski knots are constructed, which based on graph and knot theory. The growth mechanisms of them are studied and the transformation between DNA Sierpinski knots and links is realized by smoothing and restoring growing-points, some topology invariants are also presented here. Moreover, bottom-up synthesis methods about constructing DNA Sierpinski structures with minimum DNA strands are proposed.

1. Introduction

DNA is considered as an important and ideal building material in creating programmable and predictive supramolecular structure due to its special structure with two helical chains of nucleotides held together by the specific hydrogen-bonded base pairs [1]. In recent years, a large number of DNA supramolecular structures including DNA polyhedral links or catenanes [2,3] (e.g., DNA tetrahedron [4–10], DNA cube [11–14], DNA truncated octahedron [14], DNA octahedron [15–17], DNA dodecahedron [6,18], DNA icosahedron [19,20], DNA bipyramid [21], and DNA buckyballs [6]) and others [22–28] have been synthesized experimentally [29]. These structures possess significantly geometrical characters associated with polyhedra and thus arouse great interest [1,29]. It is worth noting that the majority of these structures are made up of multiple DNA strands predesigned.

[1] To whom correspondence should be addressed. Email: wyqiu@lzu.edu.cn

But recently, Li et al. pointed out that a replicable tetrahedral nanostructure can be obtained from a single-stranded DNA [10]. And Shih et al. synthesized an octahedron by folding a 1.7 kb single-stranded DNA with the help of five short DNA strands [15]. Rothemund applied the technique 'DNA origami' to assemble a long single-stranded DNA into desired shapes [30]. The results suggest that it is available to get well-defined nanostructures by folding a single-stranded DNA (ssDNA).

With the development of these exciting and intriguing results, a lot of work based on the knot theory [31,32] has been devoted to characterizing some of these amazing structures from the geometrical and topological points of view. In particular, Qiu's group put forward the methods of "*N-branches curves and M-double-twisted lines covering"* and "*N-crossing curves and M-double-twisted lines covering"* to construct polyhedral links [1,29,33–40], especially for a series of elegant DNA polyhedral links [38–40]. Meanwhile, mathematical descriptions of these structures using topology and graph theory as working tools are making great progress [41–51]. More recently, Rothemund et al. suggested that DNA can be assembled into crystals with patterns of Sierpinski triangles [52]. On the basis of this important result, we successfully designed nice DNA Sierpinski triangles, and the corresponding DNA Sierpinski links were also constructed, moreover, the growth mechanisms were studied [53]. On the other hand, an interesting issue aroused is how to construct DNA Sierpinski triangles using minimum number of DNA strands theoretically.

Our aim about this paper is to design more perfect DNA Sierpinski triangles with minimum DNA strands and to unravel the growth and transformation mechanisms of DNA Sierpinski knots. Accompany with this clear goal, we start from Euler circuit and construct a series of DNA Sierpinski knots, some formulas are aware of fulfilling the growth mechanism of DNA Sierpinski knots. Then, the operation that smooth and restore the growing-points is selected to realize the transformation between DNA Sierpinski knots and links. Finally, the methods that construct DNA Sierpinski triangles with minimum DNA strands are proposed. Our results suggest the possibility of designing DNA Sierpinski structures with minimum DNA strands, which gives a perfect access for chemists and biologists.

2. Construction of DNA Sierpinski knot

The Sierpinski triangle, the so-called Sierpinski gasket or Sierpinski sieve, is a fractal and attractive fixed set. It is described by Sierpinski through three steps [54]:

(i) begin with an equilateral triangle;

(ii) shrink the triangle to 1/2 height and 1/2 width, make three copies, and place the three shrunken triangles so that each triangle connects the other two triangles at a corner;

(iii) repeat step (ii) with each of the smaller triangles.

Shown in Figure 1 are a series of Sierpinski triangles labeled as E_0, E_1, E_2, E_3 ... E_n in order, it is readily found that they conform to the law: one grows into three, three grow into nine..., so E_n can be seen as three E_{n-1} which are connected together, and the joint points are defined as growing points, as illustrated in our previous study [53].

Firstly, a definition about Euler circuit is elaborated here.

Theorem 1: A finite graph has an Euler circuit when it is connected by odd degree without vertices. In this case, the Euler circuit can begin and end at any vertex.

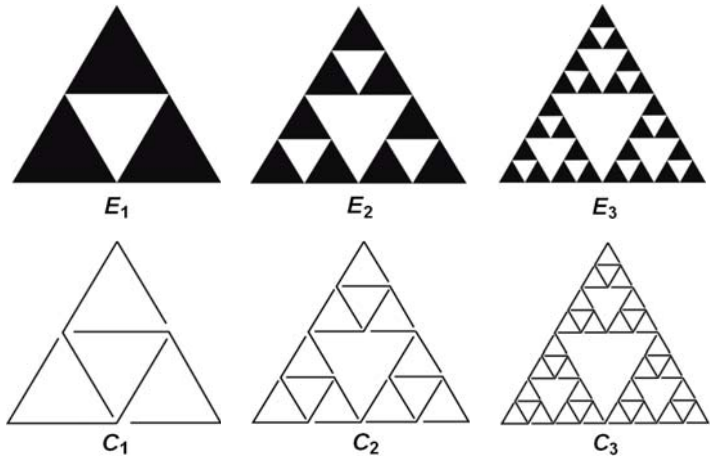

Figure 1. Sierpinski triangles E_n and their corresponding Euler circuits C_n.

If all vertices of a finite graph are even, it means that the graph has an Euler

circuit. It is obvious that a Sierpinski triangle has a homologous Euler circuit C_n when all of its vertices are even degrees. Figure 1 displays the Euler circuits of Sierpinski triangles with $n=1, 2, 3$.

Because C_n is a single walk and the crossings are under and over by turns, the Euler circuit C_n can be translated into alternating knot K_n. As a result, K_1 is a trefoil knot and K_2 can be realized by connecting three trefoil knots together by three growing points. K_3 is produced by connecting three K_2. As such, all alternating knots K_n can be obtained through the connection of three K_{n-1} by growing points, some examples are shown in Figure 2.

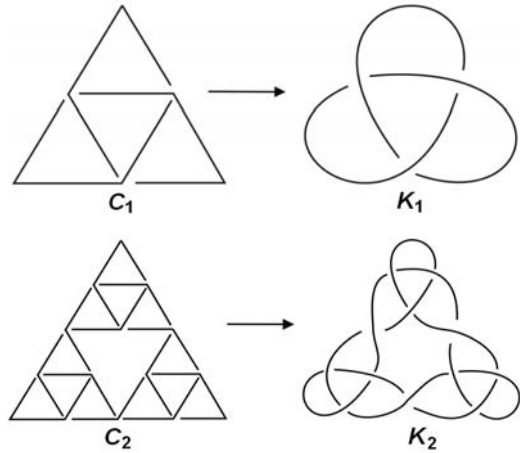

Figure 2. Translate Euler circuits C_n into corresponding knots K_n.

3. The growth mechanism of DNA Sierpinski knot

As stated above, K_n is derived from the three K_{n-1} connected by growing points. For given projections of two knots, a new knot is obtained by connecting the four terminals of the original two knots together [32]. Two cases would occur during the connection, as displayed in Figure 3 (Figure 3a indicates a crossing point appears during the connection (connection type I), while Figure 3b shows there is no crossing point during the connection (connection type II)). They may lead to

different structures.

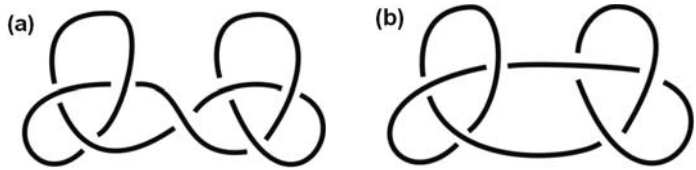

Figure 3. Two connection types of knots terminals, (a) connection type I with a crossing point; (b) connection type II without a crossing point.

For the case in Figure 3a, a knot can be obtained by connecting two trefoils together. When a more trefoil knot is added in the same way, then a new knot K_2 is obtained (see Figure 4). The new knot will always be derived by doing so. The result suggests that the ultimate structure corresponds to a knot K_n which can be connected by three K_{n-1} together. This method has something in common with DNA nanostructure synthesized by a single strand. Therefore, using this method to design and produce DNA structures with single-stranded DNA is possible.

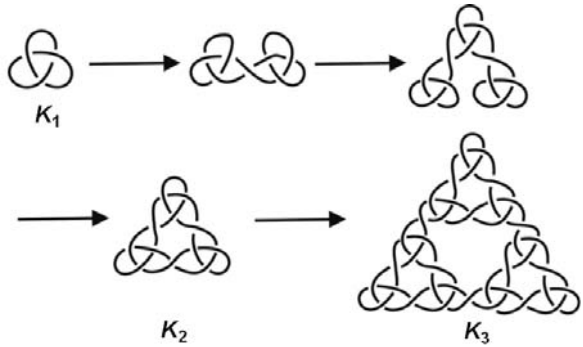

Figure 4. Scheme of constructing DNA Sierpinski knot by connection type I.

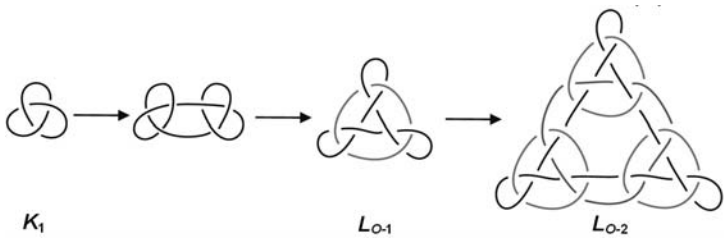

Figure 5. Scheme of constructing DNA Sierpinski link by connection type II.

Figure 5 illustrates the case without a crossing as the type II does. Similarly, starting from a trefoil, a knot can be derived by connecting two trefoils together. However, the most surprising result appears when a more trefoil is added. A DNA Sierpinski link is obtained with two components. It is easily to unravel that the link is the same as DNA Sierpinski link L_{o-1} with odd tangles, associated with the case $k=1$. Continue to construct more complex DNA Sierpinski link by connecting three L_{o-1} together, and a DNA Sierpinski link L_{o-2} with five components is got.

Repeating this operation, it can be found that the produced structures are the same as the DNA Sierpinski links with $k=1$ tangle, so the growth mechanism of DNA Sierpinski knots in the case without a crossing follows Formula (1) (see Ref.[53]):

$$A_n = \frac{3^n + 1}{2} \quad (n \geq 0,\ n \in \mathrm{Z}) \tag{1}$$

When n is zero, we get a prime knot, which also conforms to Formula (1).

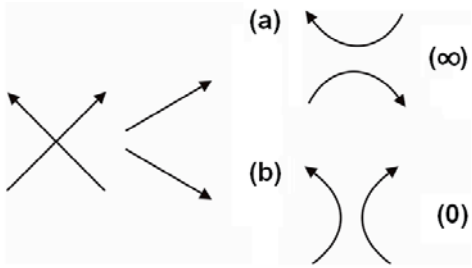

Figure 6. The operation of crossing smoothing. Converting a node into

(a) a zero configuration or (b) an infinitude configuration.

Meanwhile, it is interesting that Sierpinski knots and Sierpinski links can be interchanged with each other through the crossing-smoothing operation [32], as shown in Figure 6. In the context of DNA Sierpinski structures, it is possible to realize the crossing-smoothing operation with the help of enzymes such as shear enzymes and ligases.

Smoothing all the growing points of DNA Sierpinski knot, we can get the corresponding DNA Sierpinski link. For example, the DNA Sierpinski link L_{o-2} is

obtained by smoothing DNA Sierpinski knot K_3, as shown in Figure 7. Doing this on any Sierpinski knot, we discover that the Sierpinski knot with fractal number n is transformed into Sierpinski link with fractal number n-1. The result implies that double-stranded DNA nanostructures may be interchanged with single-stranded DNA nanostructures catalyzed by enzymes.

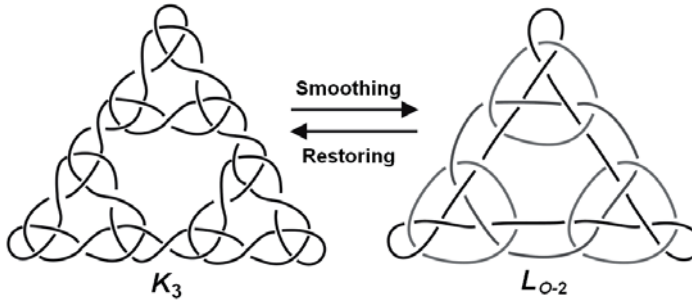

Figure 7. Interchange between DNA Sierpinski knots and links.

4. The topology invariants of DNA Sierpinski knots and links

Seifert algorithm is used here and some topological invariants are given to investigate the structure and properties of DNA Sierpinski nanostructures. The symmetry models of DNA strands are also put forward to unravel the construction rules.

(i) Seifert algorithm and some topological invariants

Seifert algorithm [55] is used to describe the surfaces featured by knots and links as boundaries. Due to the direction of DNA strands (from 5' to 3' or from 3' to 5'), the DNA strands links are oriented, and the Seifert construction can be realized by the following two steps, as shown in Figure 8.

Firstly, every crossing point is converted into the non-crossing one in the form of head-to-tail type. The resultant non-crossing circles are called Seifert circles.

Secondly, in the initial crossing points, all the Seifert circles are connected together through distorted webbings, and then the boundary of the Seifert surface

composed of links is produced. For example, a trefoil shown in Figure 9 can be transformed into two orientable circles through Seifert construction.

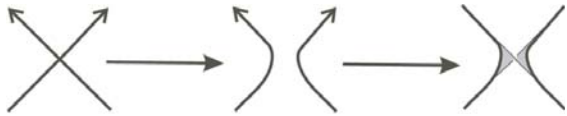

Figure 8. The operation of Seifert construction; the arrows indicate the orientation of strands.

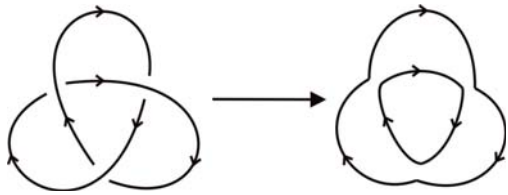

Figure 9. Seifert algorithm operates on trefoil.

Furthermore, with respect to the Seifert circles of DNA Sierpinski structures, the corresponding genus is investigated to describe the topological properties. The definition of genus of knot is illustrated below:

Definition: The genus of knot is considered to be the smallest genus in all the possible Seifert surfaces [56].

Theorem 2: The Seifert surface obtained from an alternating projection is identified to have the minimum genus [57].

All the Sierpinski knots derived from connection type I are alternating knots. Thus the genus of DNA Sierpinski knots can be calculated by Theorem 2, but the calculation is very complicate. To simplify the calculation, Theorem 3 is introduced hereafter.

Theorem 3: For a Seifert surface made up of d disks and b webbings, its genus is:[57]

$$g = \frac{1 - d + b}{2} \tag{2}$$

As shown by the example in Figure 9, the Seifert surface of a trefoil knot consists of two disks and three webbings, so the genus of a trefoil knot is 1. For an alternating knot, the webbings number b equals to twists number c, thus, the formula (2) can be changed into formula (3).

$$g = \frac{1 - d + c}{2} \tag{3}$$

And Table 1 lists the genus and some invariants of DNA Sierpinski knots.

Table1. The genus and some invariants of DNA Sierpinski knots constructed by connection type I.

Fractal number n	0	1	2	3	…	n
d	1	2	5	27	…	…
c	0	3	12	39	…	$3C_{n-1}+3=C_n$
g	0	1	4	13	…	$(3^{n-1}+1)/2$
A_n	1	1	1	1	1	1

Because the DNA Sierpinski links are connected graphs, so the genus of DNA Sierpinski links constructed through connection type II can be determined by Theorem 4.

Theorem 4: The genus of a projection surface *F* constructed from a connected diagram *D* satisfies [58]:

$$g(F) = \frac{[1 - s(D) + c(D)] + [1 - \mu(D)]}{2} \tag{4}$$

where *s(D)*, *c(D)* and *ì(D)* denote the Seifert circuit number, crossing number and component number of connected graph, respectively. The genus and some invariants of DNA Sierpinski links are listed in Table 2.

Table2. The genus and some invariants of DNA Sierpinski links constructed by connection type II.

Fractal number n	0	1	2	3	…	n
s(D)	1	2	5	14	…	$3s_{n-1}(D)$-1
c(D)	0	3	9	27	…	3^n (n≥1)
μ(D)	1	1	2	5	…	$(3^{n-1}+1)/2$
g(F)	0	1	2	5	…	$(3^{n-1}+1)/2$

Tables 1 and 2 show that the genus of the Sierpinski structures, which is a function of fractal number *n*, indicating that the genus is an intrinsic character of Sierpinski structures. The properties of Sierpinski structures are determined by the genus. It is shown that the genus is increasing with the fractal number *n* (see Tables 1 and 2), so the character of DNA Sierpinski structures with different fractal number *n* is similar to each other.

(ii) The designing rules of DNA strands

To elaborate the designing rules of DNA strands, DNA strand models obtained from the analysis DNA Sierpinski structures using graph theory are represented below.

First of all, the *step length l* as defined in the previous study [53] is employed. For an alternating links or knots, the step length is the length from one up-crossing point (or down-crossing point) to the next up-crossing point (or down-crossing point). The full step length is the sum of step length of a DNA strand, the longest DNA strand is indicated by l_{max}.

With regard to the DNA Sierpinski knots, supposing that the length of each edge of DNA Sierpinski knot is $0.5a$, so it can be found that the step length of DNA strands has the following distribution:

$n = 1, 1.5a + 1.5a + 1.5a;$

$n = 2, (a)_3 + 1.5a + (a)_3 + 1.5a + (a)_3 + 1.5a;$

$n = 3, (a)_{12} + 1.5a + (a)_{12} + 1.5a + (a)_{12} + 1.5a;$

...

It suggests that $(a)_q$ is a repeated unit between $1.5a$ and $1.5a$. The value of q increases by a regular rule that satisfies formula (5), so the DNA strands model can be explained by Figure 10a. Investigating the step length distribution of DNA Sierpinski links, the DNA strands model is shown in Figure 10b.

$$3q_n + 3 = q_{n+1} \quad n \geq 1, n \in Z \quad q_1 = \tag{5}$$

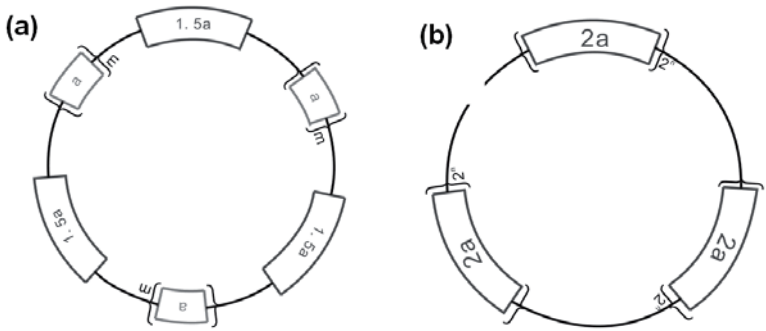

Figure 10. The models of DNA strands that formed DNA Sierpinski knots and links.

(a): strands model of DNA Sierpinski knots; (b): strands model of DNA Sierpinski links.

5. Investigation of the synthesis method

Two bottom-up synthesis methods of DNA Sierpinski triangles based on the constructed structures are proposed.

With regard to any Sierpinski knots, for example, as shown in Figure 11, every Sierpinski triangle can be divided into three identical parts, which can be divided into smaller and smaller parts until the smallest building block shown in top right of figure 12. It is very similar to Seeman's original strategy of synthesizing DNA polyhedra [59].

Then we can design single stranded DNA on purpose and assemble them into the smallest building blocks. Finally, the desired DNA Sierpinski knots can be realized through reverse synthesis strategy. If the single stranded DNA or RNA structures are synthesized in labs, it not only produces new DNA nanostructures but also provides dramatic ideas and opportunities for duplication and transcription of DNA nanostructures. As to DNA Sierpinski links, a certain number of various DNA strands are prepared and folded into circles and then assembled into desired links with the aid of enzymes.

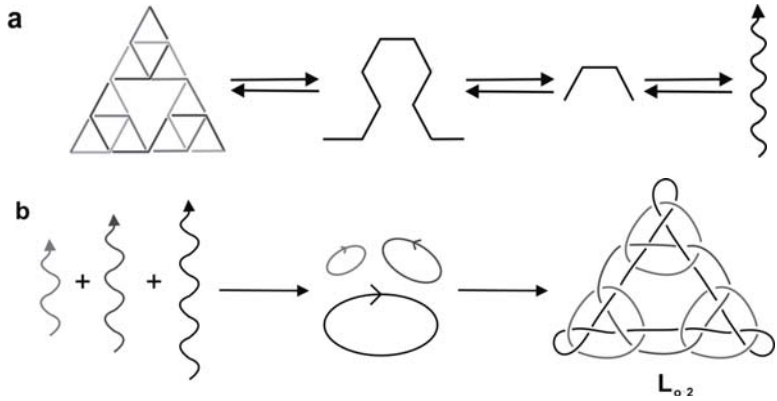

Figure 11. Schemes of synthesizing DNA Sierpinski knots and links.

The first method has advantage for small structures. If the targets are big and more complex, then more different DNA strands are needed, it is a huge work to complete by the first method. So the other method that synthesized DNA Sierpinski

knots and links from the chosen basic building blocks with the help of enzymes such as DNA shear enzymes and ligases is needed. The DNA trefoil knots are selected as the basic building block and vertexes of them are unlocked. Three unlocked DNA trefoil knots are connected together by special ligases at the three growing points. If they are connected by connection type I, we get knots, otherwise, the result is a link by connection type II. All DNA Sierpinski knots and links can be synthesized through this method.

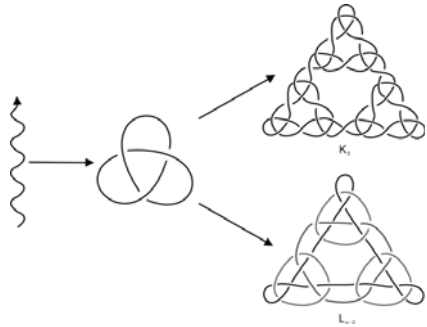

Figure 12. The strategy of synthesize DNA Sierpinski knots and links from basic building block.

6. Conclusion

Although DNA nanostructures synthesis is growing vigorously, the designing and investigation of DNA nanostructures is in its infancy. In these paper, new synthesis strategies about DNA Sierpinski knots was presented through mathematic methods.

The Euler circuits about Sierpinski triangles were explored and then changed into Sierpinski knots. Sierpinski knots and links were constructed from the smallest Sierpinski knot trefoil knot and the growing mechanisms were also investigated. A straightforward proof about the possibility that DNA Sierpinski knots can be translated into DNA Sierpinski links with help of enzymes is presented. We also put forward two bottom-up synthesis methods based on the growing mechanisms of Sierpinski knots and links.

Our research on DNA Sierpinski structures is elementary, especially on fractal structures, but these superficial results may help us to open the door of analysis and

simulate fractal super-molecular and viruses with mathematic models. New ideas are input in the duplication and transcription of DNA nanostructures, the theory of DNA nanostructure is supplemented and became more perfect.

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