Orderly Branched Tangles Based on Carbon Nanotube Inspired by Grossman's Sculptures

Hou-Hsun Ho[1] and Bih-Yaw Jin[2]

Department of Chemistry, National Taiwan University, Taipei, Taiwan
[1]d10223105@ntu.edu.tw, [2]byjin@ntu.edu.tw

Abstract

We develop a procedure to design complex tubular branched tangle structures based on curved and branched carbon nanotubes (CNTs). A curved CNT is obtained by mitering CNT segments, and a branched CNT can be generated by puncturing a generic fullerene in line with its specific symmetry. With curved and branched CNTs as basic building blocks, we can construct a wide range of hypothetical molecular structures with arbitrary space curves based on CNTs. Following the procedures given above, we show CNT versions of Bathsheba Grossman's Metatron and Metatrino sculptures and present the corresponding beaded model of Metatrino.

Introduction

Ora, Metatron, Metatrino, Quintron, and Quintrino are mathematical sculptures designed by Bathsheba Grossman. They are orderly branched tangles with regular polyhedral symmetries [2]. The Metatron and Metatrino can be viewed as a cube and a regular octahedron, respectively, and are the dual of each other. Similarly, the Quintron and Quintrino belong to the dodecahedron and icosahedron categories. Ora, analogous to a regular tetrahedron, is self-dual. In these mathematical sculptures, the faces of parent polyhedra are converted to branched nodes (face nodes), which are then connected to the vertices on the original faces, also converted to branched nodes (vertex nodes). The number of edges is doubled under such operation and the links between the face and vertex nodes are curved to avoid the interpenetration.

Considering the geometry of these sculptures which bear some resemblance to our previous works on the CNT based polylinks [3], we ask a question about the possibility of creating a graphitic representation of these orderly branched tangles designed by Bathsheba Grossman by decomposing the complex structures into two basic units: the branched and curved tubular joints. The present article is organized in the following manner. Firstly, we establish the construction scheme for curved CNT by systematically mitering mirror-image CNT segments. Secondly, we demonstrate the approach to generate branched CNT by puncturing fullerenes, the spherical counterpart of CNT. Finally, the curved and branched CNTs are integrated to build the branched tangle structures.

Curved Carbon Nanotube

In our previous work in Bridges [3], we demonstrated that we could make a bent tube by mitering the mirror-reversed (n, m)-(m, n) CNTs, where (n, m) is the chiral vector of a CNT. The bending angle of CNT depends on the chiral vector [5]. This is illustrated in Fig.1, where a (2,5)-(5,2) bent CNT is represented as a band of honeycomb lattice with a pencil-shape cutout (left shaded area). The 3D structure of the bent CNT can be obtained by joining the two sides of the cutout as well as the top and the bottom of the band, essentially creating a dislocation at the center of the cutout area. This corresponds to introducing a pentagon-heptagon pair in the honeycomb band which would otherwise be a straight tube when joined. Furthermore, we can miter bent CNT consecutively to get a CNT resembling an arbitrary space curve [6]. To do so, we start by introducing a second dislocation as shown in Fig.1(a) (right shaded area). Apparently, the placement of the second dislocation is not unique. We could shift the second dislocation to alter its relative position, making the second bend at an angle with respect to the first one. The arrows in Fig.1(a) indicate a set of possible shifts, and the shifting procedure is parametrized by a pair of integers (vs, hs), see [3] for a detailed description. From the aspect of tubular structures, the shifting of dislocation results in torsion (dihedral angle rotation) and change of separation between adjacent corners. Since curvature (bending) and torsion (dihedral angle rotation) are the fundamental properties of space curves, we can simulate a wide range of space curves based on CNT by systematically shifting each segment, as shown in Fig.1(b) [6].

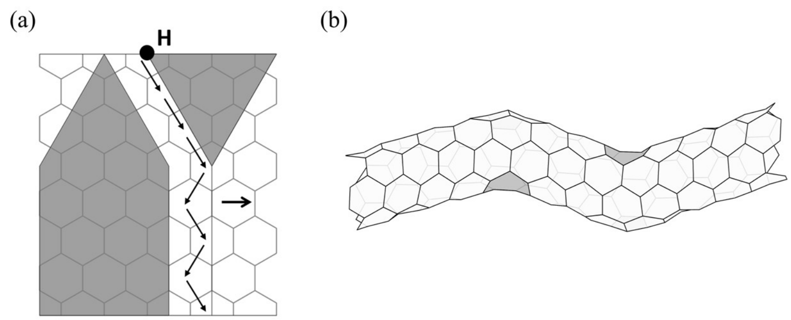


Figure 1: *Diagrams that represent consecutive junctions of bent CNT which change the relative positions of adjacent dislocations and the outcoming curved CNT. (a) The second dislocation is placed next to the first one with the tip pointing down. The black dot H indicates the position of the heptagon, and the arrows imply practical shifting directions. (b) A curved CNT from consecutively mitering CNT segments. The dihedral angle between the corners is specified by the relative position of adjacent dislocations.*

It is useful to estimate the dihedral angle of a given (vs, hs) pair. Empirical results indicate that the dihedral angle between CNT junctions with $(vs, hs) = (1,0)$ is approximately π regardless of the chiral indices (n, m) of the tube. Based on this observation, we start by drawing the projection of the CNT axis on the honeycomb band (blue line in Fig. 2) that is perpendicular to the circumference vector (thick black line) of length D. The blue line passes through $(1,0)$, indicating that all lattice points (vs, hs) which are on the line give rise to a dihedral angle of π between the two bends. For other cases the dihedral angle ϕ deviates from π, with the magnitude of the deviation proportional to the ratio between the point-line distance d and the circumference D

$$\phi = \pi\left(1 - 2\frac{d}{D}\right),$$

where the factor of two comes from the periodic boundary condition across the band (the top and the bottom horizontal lines).

The bending angle and the dihedral angle are defined by (n, m) and (vs, hs) respectively. One can therefore build a specific discrete curve on demand through searching the space of these discrete parameters.

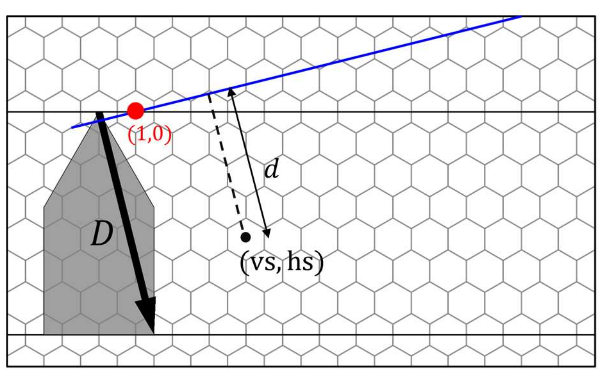


Figure 2: *Diagram of the dihedral angle of certain (vs, hs) pair. The blue line is the projection of the corresponding CNT axis passing through $(vs, hs) = (1,0)$, the case where the dihedral angle is π.*

Branched Carbon Nanotube

The previous work by Jin et al. [4] demonstrates that a branched CNT junction can be obtained by puncturing holes on a fullerene (a polyhedron with pentagonal and hexagonal faces) and joining them with tubes of suitable radii. Following that work, we first choose a particular fullerene based on the symmetry requirement of the branched CNT. For instance, to get a triply branched CNT as shown in Fig.3(d), we start from the fullerene in Fig.3(a) with threefold rotational symmetry. We identify the locations (the red dots) from which the tubes emerge. The red dots are then eliminated to prepare for the junction of tubes, as shown in Fig.3(b) and Fig.3(c). Finally, we obtain a triply branched CNT in Fig.3(d) with threefold rotational symmetry. Following similar steps, we can generate a hollowed quadruply branched CNT in Fig.3(f) from puncturing the surface of a fourfold rotational symmetric toroidal carbon nanotube in Fig.3(e) [1].

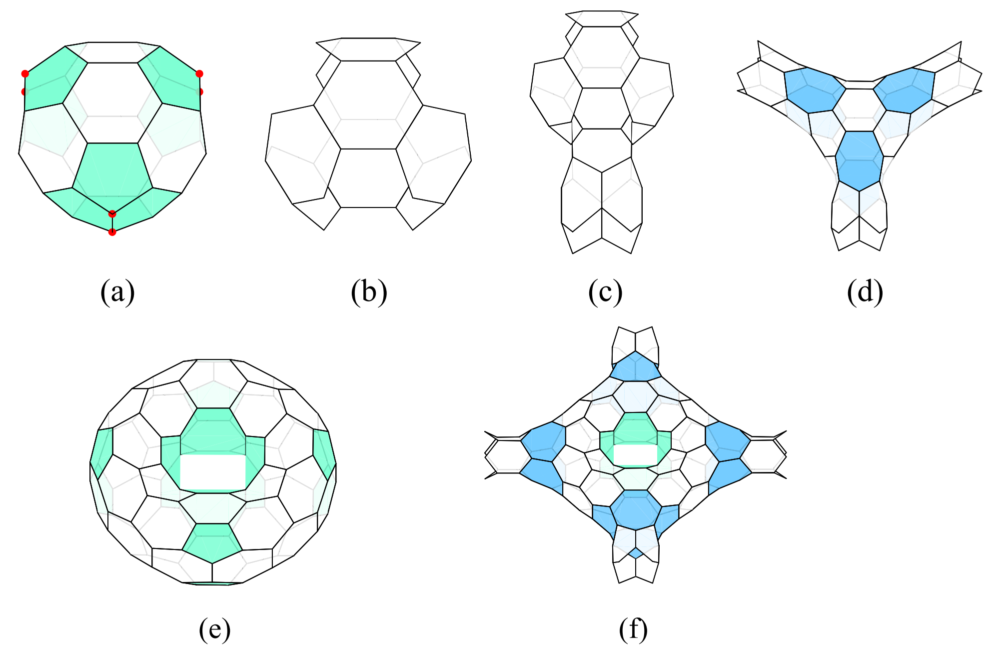
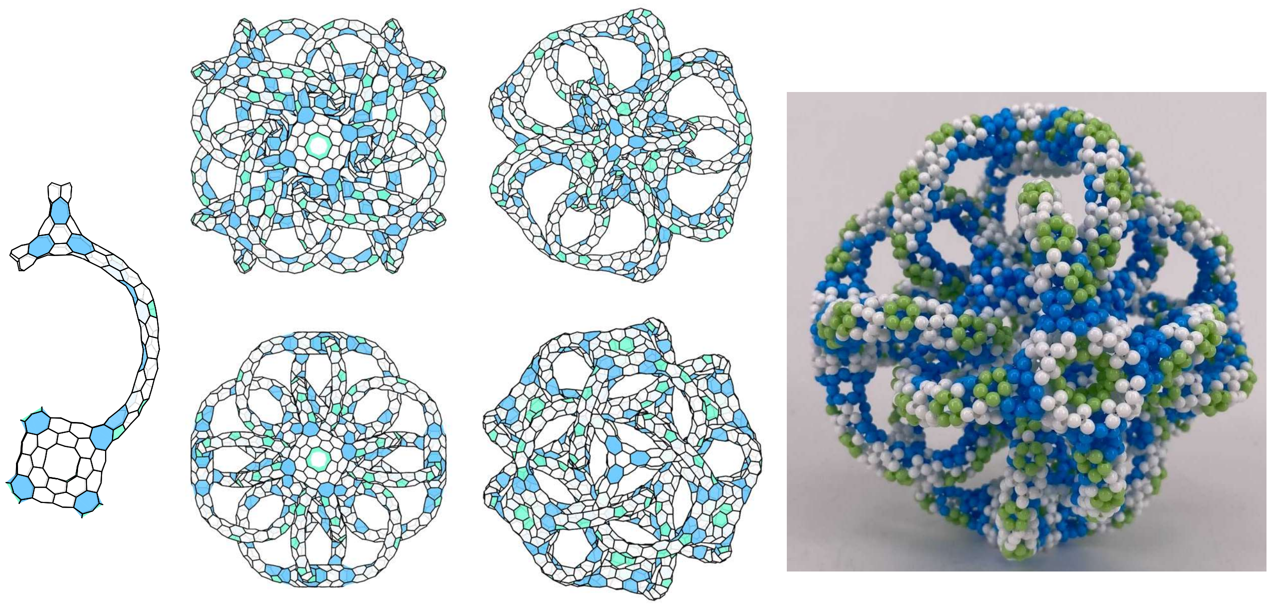


Figure 3: *The process of constructing a triply branched CNT starting from a fullerene. (a) A fullerene with threefold rotational symmetry. (b) The fullerene is punctured with red dots on (a) eliminated, which are the locations where CNT emerges. (c) CNT with a proper radius is joined onto the hole, with each vertex remaining connected to three other vertices. (d) The resulting triply branched CNT with six heptagons (blue). (e) A toroidal CNT with fourfold rotational symmetry. (f) The corresponding hollowed quadruply branched CNT.*

Complex Space Curve Design with CNT

With curved and branched CNT as building blocks in hand, we can construct diverse designs of tubular structures by combining them systematically. Here, we demonstrate our designs of Bathsheba Grossman's Metatron and Metatrino sculptures based on this strategy. The hollowed quadruply and triply branched CNT in Fig.3 are respectively used as the face and vertex nodes, and they are linked with curved CNT. The basic unit of the complex structure is shown in Fig.4(a), which is composed of a triply branched CNT, a segment of curved CNT, and a hollowed quadruply branched CNT. The rendering CNT structures of Metatron and Metatrino are shown in Fig.4(b) and Fig.4(c), and Fig.4 present the beaded model of Metatrino, which took us about 50 hours to construct.



(a) (b) (c) (d)

Figure 4: *(a) The basic unit of the complex structure. (b) The CNT versions of Bathsheba Grossman's Metatrino (top) and Metatron (bottom) sculptures viewed from the 4-fold axis. (c) The CNT versions of Bathsheba Grossman's Metatrino (top) and Metatron (bottom) sculptures viewed from the 3-fold axis. (d) The beaded model of the Metatrino based on CNT.*

Acknowledgements

We thank the Ministry of Science and Technology, Taiwan, for financial support.

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