Constructing Bead Models of Smoothly Varying Carbon Nanotori with Constant Radii and Related Intersecting Structures

Hou-Hsun Ho[†1], Chern Chuang[‡], and Bih-Yaw Jin[†2]

[†]Department of Chemistry, National Taiwan University, Taipei, Taiwan
[‡]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada
[1]b06203004@ntu.edu.tw, [2]byjin@ntu.edu.tw

Abstract

We develop a systematic procedure to construct models of carbon nanotori with smoothly varying local curvature. The tubular radius is preserved by repeatedly connecting a tube with its mirror image and forming a torus, where a set of five indices suffice to uniquely characterize this scheme. We also extend the constructing strategy to stadium- and star-shaped rings and the corresponding intersecting structures. The bead models of the structures are presented as well.

Introduction

The graphitic system, the collection of sp^2 carbon allotropes, has raised attention for its fascinating physical properties. Apart from its possible applications, we are highly interested in such systems because the triply connected graphs can be realized particularly well by bead models, where the beads are related to the edges of the mesh. As part of the class, carbon nanotubes (CNTs) are straight tubules obtained by rolling up a graphene, a honeycomb of carbon atoms. The geometry of a CNT can be uniquely defined by its chiral vector, the boundary condition of CNT, a two-component vector relating two honeycomb lattice points.

As a derivative of CNTs, carbon nanotori are tubular loops with genus one surfaces. In 2009, Chuang et al. epitomized various types of carbon nanotori by elegantly performing manipulations on the tiling of a hexagonal hollowed prism [1]. Some of the nanotori, however, look like rounded polygonal rings rather than circular tori with smoothly varying curvatures. This is ascribed mainly to the high density of defects (pentagons and heptagons) in a single junction. In this work, we introduce a strategy to generate nanotori with smoothly varying curvature and constant tubular radius. It is worth mentioning that this type of torus is not beyond the scope of Chuang's research; nevertheless, we view the constructing procedure from a distinct viewpoint which enables us to build various shapes of rings with constant tubular radius.

Carbon Nanotori

In the first place, we demonstrate the approach for generating carbon nanotori by mitering nanotubes consecutively. Given a chiral CNT with chiral indices (n, m), we could connect a pair of mirror-reversed (n, m)-(m, n) CNTs by carefully inserting a pair of pentagon and heptagon into the tubular system [2]. First, we cut the pencil-shaped dislocation $PHP'P'H$ out of the graphene sheet in Fig.1a. The two $\overrightarrow{PH}$ vectors on the tip of the pencil are specified by $(n-m, 0)$ and $(0, n-m)$, and the $\overrightarrow{HP'}$ vectors on the shaft part of the pencil are denoted by (m, m). Fusing both PHP' sides together leads to a dislocation containing a pair of defects in Fig.1b. We then roll up the strip of graphene to the tube in Fig.1c, which represents the radius-preserving CNT junction with a mirror plane passing through the midpoint of two defects.

Due to the positive and negative curvatures accompanying the corresponding pentagon and heptagon, the tube deforms with a specific bending angle, illustrated in Fig.1c. Besides, the vectors connecting the pentagon and the heptagon at the joint are uniquely determined by the chiral indices of the tube (in this case, $(3,0)$ and $(2,2)$). It is noteworthy that this kind of junctions is the only way to preserve the tubular radius and contains exactly one pair of defects at the same time. Other ways to create a junction either change the diameter or introduce extra pairs of defects [2].

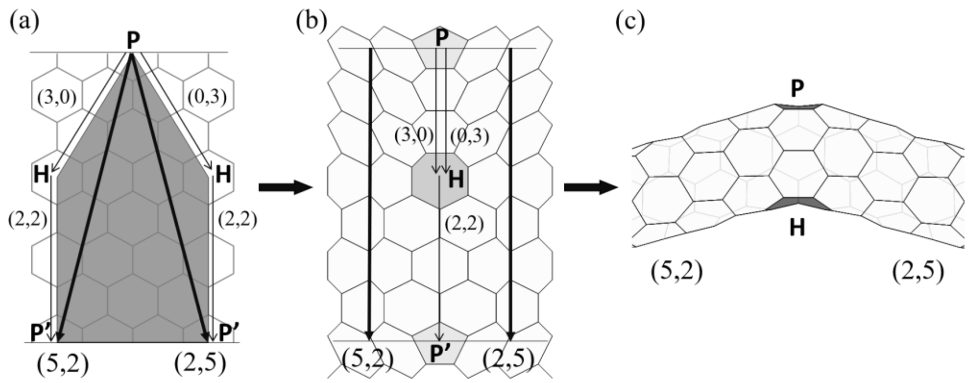


Figure 1: *Three steps of connecting chiral CNT with its mirror image (5,2)-(2,5). (a) Cutting off a dislocation (grey area) and fuse two sides to generate a pair of defects in (b). The sheet is then rolled up to form a bending tube in (c).*

Roughly speaking, repeatedly joining such junctions creates a torus. To get a continuously bending tube, we place a second dislocation in the opposite way to switch back the chirality of the graphene sheet as shown in Fig.2a. Apparently, this choice is not unique. We could, in general, apply vertical shift (Fig.2b, left) and horizontal shift (Fig.2b, right) to the second one to alter its relative position. To specify the shifts, we focus on the black dot **H** on the second dislocation in Fig.2, which is the position of heptagon and able to represent each unique dislocation. Furthermore, the grids are parametrized by the vertical and horizontal shifts (vs, hs) as shown in Fig.2c. We note that (vs, hs) does not follow the usual convention of chiral indices. However, this definition affords a bijective correspondence between all possible shifting states and nonnegative integer pairs $(1 \leq vs \leq n+m, 0 \leq hs)$. After elaborating the placement of the second dislocation, the two dislocations can be viewed as a unit. A torus is obtained by duplicating the unit *N* times to miter the tubes repeatedly as depicted in Fig.3, where *N* is the rotational symmetry number of the torus.

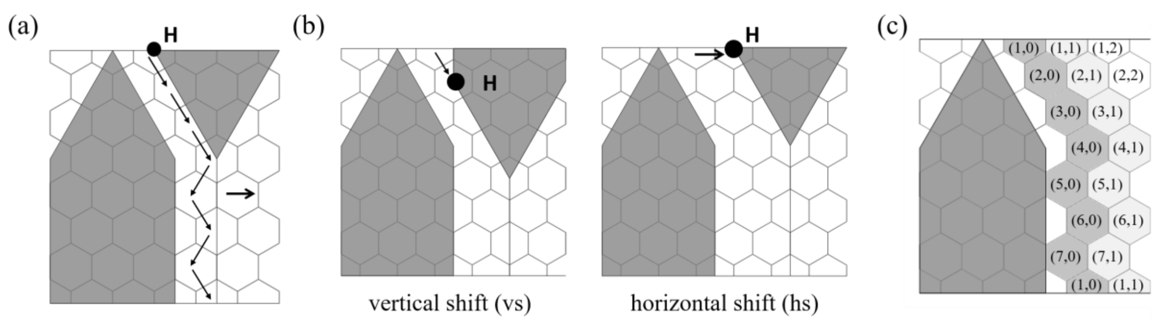


Figure 2: *Diagrams that represent consecutive junctions and the operations which change the relative displacement of adjacent dislocations. (a) The second dislocation is placed next to the first one with the tip pointing down. The black dot H indicates the position of heptagon and the arrows imply practical shifting directions. (b) The left one shows the vertical shift (vs) for H as it descends along the edge of the first disclination. The right one demonstrates the horizontal shift (hs) for H as it moves horizontally along the row of hexagons. (c) Possible positions of H parametrized by (vs, hs). The linear independent operations span the strip of graphene.*

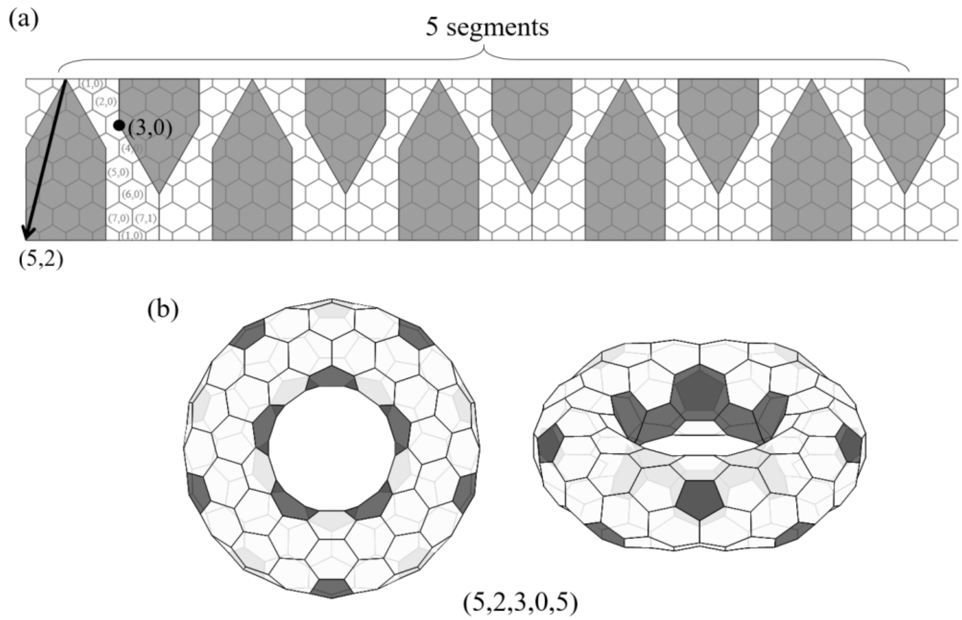


Figure 3: *Constructing carbon nanotori by repeatedly connecting tubes, and the structure can be fully described with five indices (5,2,3,0,5). (a) Conjugated dislocations mapping on the graphene. (b) The corresponding carbon nanotori after the cut and paste procedure from (a).*

The geometrical information of the torus can be fully described by five indices, which determine the chiral vector of the tube (n, m), the relative position of two adjacent dislocations (vs, hs), and the number of segments (N). By removing the shaded pencil-shaped area and gluing edges suitably, Fig.3a can then be transformed into Fig.3b, a carbon nanotorus with indices (5,2,3,0,5).

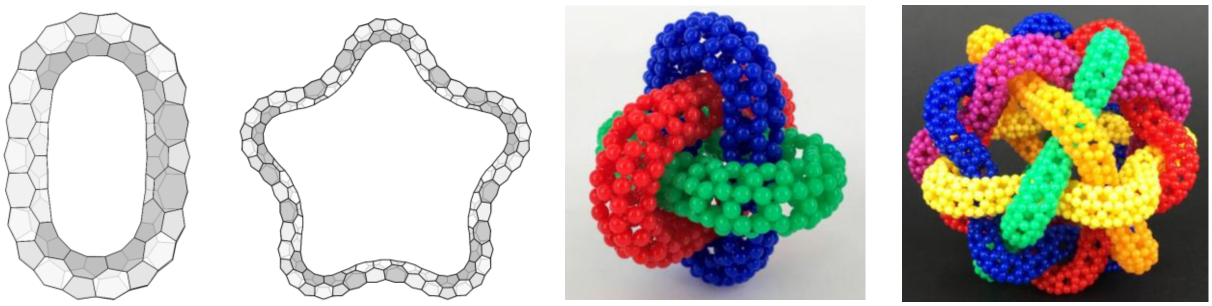
Following the construction scheme of smoothly varying carbon nanotori above, we present the pictures of beaded tori in Fig.4, in which the beads take the position of edges of the structures shown above. The defects (five- and seven-membered rings) are represented by colored beads with the remaining beads on regular six-membered rings being white. It is evident that these discretized toroids have smoothly varying curvature and are close to ideal circle-shape tori, as compared to a large family of tori covered in Chuang's classification scheme previously, with a representative torus shown in Fig.4d.

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

Figure 4: *(a), (b), and (c) are the bead models of carbon nanotori with the geometrical indices being (3,1,4,0,10), (3,2,4,0,9), and (3,2,2,0,10), respectively. (d) Chuang's polygonal torus.*

Different Shaped Carbon Nanoring and Related Structures

Apart from regular toroidal systems, we extend the mitering procedure to form more flexible tubular structures. Inspired by the concept of space curve design of discretized segments developed by C. H. Séquin et al. in 2019 [3], we treat each junction as a bending module and rotate the dihedral angle between two corners by manipulating the vertical and horizontal shifts. Theoretically speaking, by this means it is almost possible to build up an arbitrary tubular space curve. However, finding the proper shifting of each unit for a specific curve is indeed grueling, which we can currently achieve by trial and error. Therefore, we only demonstrate two structures we have successfully completed and the related artistically pleasing bead crafts.



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

Figure 5: *(a) Stadium-shaped carbon nanoring. (b) Star-shaped carbon nanoring. (c) Bead model of Borromean rings formed with three units in (a). (d) Bead model of orderly tangled six star-shaped rings.*

Here in Fig.5a is a stadium shaped carbon nanoring with C_{2h} symmetry. A pair of semi-circles are connected via two short segments of nearly straight CNTs, each with five consecutive dislocations. Fig.5c is the corresponding bead model of CNT based Borromean rings made up of three stadium-shaped nanoring. Although none of the rings are linked with each other, the overall structure cannot be separated. Moreover, the length of the link between two semi-circles in one ring is adjusted to precisely accommodate the insertion of another perpendicular ring in order to avoid loose packing of the whole compound. In Fig.5b, a star-shaped carbon nanoring is presented. It is constructed by connecting two types of arcs alternatingly, ones with smaller radii facing inward while the others facing outward. We handle the connection between two parts attentively to prevent deviation from the plane of the star. The regular polylink consists of six star-shaped rings is shown in Fig.5d. The six components lying on the great circle of the corresponding icosidodecahedron are orderly tangled [4]. We also accurately regulate the lengths of the two arcs to achieve a nearly tight configuration.

Acknowledgements

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