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Optimizing Energy Configurations in the Formation of Hybrid Carbon Nanocone–Nanotorus Structures

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Abstract: The production process of hybrid nanostructures such as cones and torii facilitates the development of advanced nanoscale technologies. This study minimizes two curvature-dependent energies to model the ideal junction between a nanocone and a nanotorus. We propose a geometric and analytical framework to construct such junctions along with computations in order to demonstrate the alignment of boundaries and gradients. The results indicate a physically significant and energetically advantageous local connection, offering insights into the creation of hybrid carbon nanostructures for prospective nanoscale applications. In particular, we obtain two continuous smooth transitions in 2D and 3D scenarios among the proposed nanostructures resulted from elastic energy and helicoid surface respectively. These approaches can be extended to include other nanostructures, thereby increasing the potential use of nanoscale devices in these fields such as nanofluidics and nanoelectronics.

Keywords: Energy minimization, curvature-dependent, Helicoid, Nanotorus, Nanocone

1 Introduction

Carbon nanostructures possess exceptional characteristics that set them apart from other material structures. Due to these characteristics, they are outstanding candidates for the production of hybrid structures. Hybridization defines as the geometric joining of two distinct carbon nanostructures into a single continuous surface, rather than to electronic or chemical orbital hybridization. These combined structures produce integrated properties, resulting in general enhancements of the original physical and chemical properties.
Ge and Sattler first discovered carbon nanocones in 1994. These are composed of a graphene sheet featuring a pentagonal disclination. Such structures have various applications across multiple fields due to their conformation properties; they are used in energy devices, biomedical applications [1,2,3,4], thermal rectifiers [5, 6], and even photovoltaics and supercapacitors [7,8]. According to Eulers theorem, a carbon nanotubes cap can be formed with six pentagons. Therefore, the possible cone angles are 180°, 112.90°, 83.60°, 60°, and 38.90° [9].

Another interesting form of carbon nanostructures is the carbon nanotorus. This shape can be created by joining the two ends of a folded carbon nanotube. It exhibits considerable properties, which makes it useful in various applications. These include its chemical and physical stability, large magnetic moments, high magnetic response, and high reversible tension [10,11,12]. Mainly it might be a generator for gigahertz frequencies [13], which make it helpful in ultra-fast filters and powerful electromagnetic signal detection in nanoantennae [14]. In addition, it might be employed in several purposes including chemical chains, encapsulate atoms, nanoelectromechanical systems and nanoparticles into its inner cavity [15,16].

In contrast of carbon nanostructures that used in classical sp^2-hybridization such as nanotubes, graphene and fullerenes, grapgynes offer an interesting type of carbon materials which demonstrate a combination with $sp - sp^2$ hybridization. Their configurations involve of hexagonal carbon structures joined by acetylenic bonds leading to special mechanical, structural and electrical features compared to graphene. Consequently, graphynes have been thoroughly investigated for promising uses in various fields for example, technologies for membrane

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filtration, energy storage and nanoelectronics.

Numerous researches have examine graphynes structures and characteristics. specifically, transport advantages, electronic band systems and mechanical dynamics [17,18]. In a thorough review of graphyne by Belenkov et al., graphyne polymorphs were studied to underline their structural stability and possibility of other carbon nanostructures hybridization [19]. Furthermore, 48 graphynes composite of graphene have been provided in recent investigations, which similar to Schwarzite in structures with distinct mechanical and electronic features [20]. Because of their capability in different topological surfaces production, integration graphyne structures into hybrid carbon nanostructures might offer novel viewpoints on surface simulation and energy efficiency.

Although both graphene and graphynes have same structures, graphynes structures in $sp-sp^2$ hybridization produces localized curvature implications which affected the hybrid nanostructures construction. Future research might examine if graphyne-based configurations could benefit from the same energy-based approaches used for nanotube junctions, Schwarzites or minimum surface techniques.

Numerous prior studies have investigated the production of hybrid structures among carbon nanostructures due to their potential applications as in microscopy, administering medicines and energy store [21,22]. Consequently, different mathematical techniques have been explored to describe this method.

The determination of the conjoining region between nanostructures resulted from the Euler-Lagrange equation which is calculated using variational calculus is one of the attractive method of this issue, as reported by Cox and Hill[23]. That is reducing the curvature square to simulate nanostructures, a technique called the elastic energy approach. According to technique, several hybrid configurations have been created such as two tubes [24], graphene-tube [23], tube-cone [9], and others as presented in [25].

Another solution applied in the literature to distinguish the connection area entails counting the rotational curvature as well. This is called the Willmore energy approach and is considered a natural generalization of the previous model. This energy has significant importance in various scientific applications, including nanotechnology and molecular biology [26,27, 28]. Consequently, the connection area has been modelled using an absolute minimizer surface with a mean curvature equal to zero. Thus, the catenoid surface has been used for this purpose, as shown in our previous research [29]. As a result, various 3D hybrid structures have been generated such as tube-fullerene, fullerene-fullerene [29], and tube-torus [30].

Although many studies have examined the use of a catenoid surface to merge materials in nanoscale, there is limited investigation on the influence of other absolute minimizers of Willmore energy in hybrid creation process. Besides, no research made to join both structures: carbon nanocones and carbon nanotori by employing elastic energy.
Helicoid surfaces were first presented in 1842 by Catalan, who defined these surfaces as twisted flat planes revolving around their central axis, as depicted in Figure 1 [31,32,33]. Recognized for their zero mean curvature,

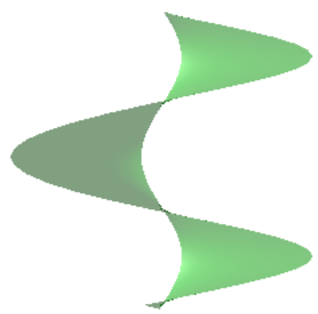

Fig. 1: An example of a helicoid surface.

helicoids are identified as minimizers of surface energy. This characteristic enables advantageous applications in minimal energy configurations, such as nanostructure modelling and soap film formations [33]. The purpose of this study is to produce a smooth conjoining between a carbon nanotorus and a carbon nanocone by utilizing a helicoid surface which identified as minimizer for elastic and Willmore energies.
The present study proposes a model for hybrid nanostructures production using helicoid surfaces. Also, it expands the application of elastic energy to cover nanotori-nanocones conjoining. This model reduces the energy of curvature, simplifying the basics in nanostructures production that is usable in nanoscale manufacturing processes. Finally, the findings help to increase our understanding of minimum surface applications in the nanomaterials production.
The basic equations for modeling the connecting area between nanostructures are introduced in the next section. The results of producing hybrid structures using the

previously discussed models are incorporated in Section 3. The paper finally concludes in Section 4.

2 Mathematical models

2.1 Willmore energy function approach

The energy here takes into account both curvatures, the axial κ_a in addition to the rotational κ_r, that is defined as:

$$J_w[y] = \int (\kappa_a + \kappa_r)^2 d\mu + \lambda \int d\mu, \quad (1)$$

with area element $d\mu$ and a Lagrange multiplier λ. We suppose the surface for the joining as $(r\cos\theta, r\sin\theta, f(r,\theta))$. As a result a surface satisfies $H = 0$ is a complete Willmore energy minimizer. Therefore, the addition of both curvatures gives

$$\frac{f''(r)}{(1+f'^2(r))^{\frac{3}{2}}} + \frac{f'(r)}{r\sqrt{f'^2(r)+1}} = 0.$$

For which the general solution can be written as

$$f(r) = \pm\frac{1}{A_1}\log(A_1 r) + A_2. \quad (2)$$

The function represents the surface of a helicoid; constants A_1 and A_2 are used. Specifically, the positive sign indicates that the helicoid spirals upward, while the negative sign indicates a downward spiral, as shown in Figures 2 and 3.

Consequently, a helicoid will be used as the joining surface between the nanocone and nanotorus, as demonstrated in Figure 4. For additional and relevant mathematical derivation, please refer to [29].

2.1.1 Geometry of structures

Now, we are going to describe the mathematical parametric equations for the helicoid, cone, and torus. First, we can identify the helicoid in cylindrical coordinates using the following parametric equations:

$$S = (x,y,z) : r\cos\theta, r\sin\theta, c\theta,$$

where c is the twist rate, r is the radial parameter and θ is the angular parameter. Furthermore, the parametric equations for the cone are

$$S = (x,y,z) : r\cos\theta, r\sin\theta, r\left(\frac{h_c}{r_c}\right), \quad (3)$$

where h_c is the cones height, r_c is the radius of the base and r is the radial distance from the apex to the base. In addition, the torus expands as:

$$S = (x,y,z) : (R_t + r_t\cos v)\cos u, (R_t + r_t\cos v)\sin u, r_t\sin v, \quad (4)$$

where R_t and r_t are the major and minor radii respectively.

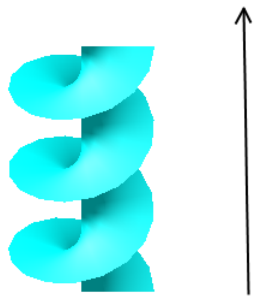

Fig. 2: Directions of the helicoid twist: positive twist

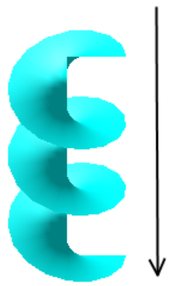

Fig. 3: Directions of the helicoid twist: negative twist

2.2 Calculus of variations energy approach

In this section, we determine the basic variational equation for the merging among carbon nanocone and nanotorus. The position of the nanocone is assumed as that the origin of the (x,z)-plane is where the cone vertex is situated with base radius r and cone angle ψ. The location of the nanotorus with radius b_2, angular position γ, major radius R and minor radius r_1 is at a distance y_0 over the (x,z)-plane, with its axis colinear with the y-axis. We may address this as a 2D case in the plane of xy as both nanostructures display rotational symmetry around

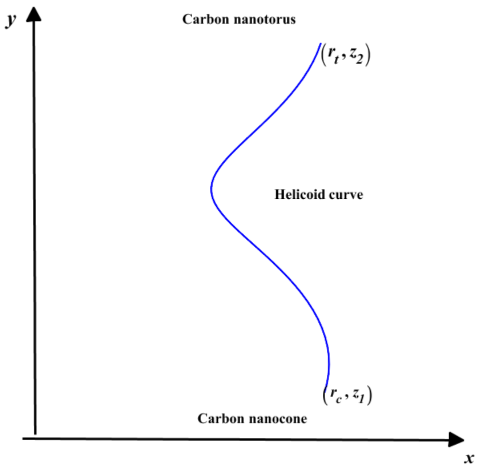

Fig. 4: Joining configuration using helicoid.

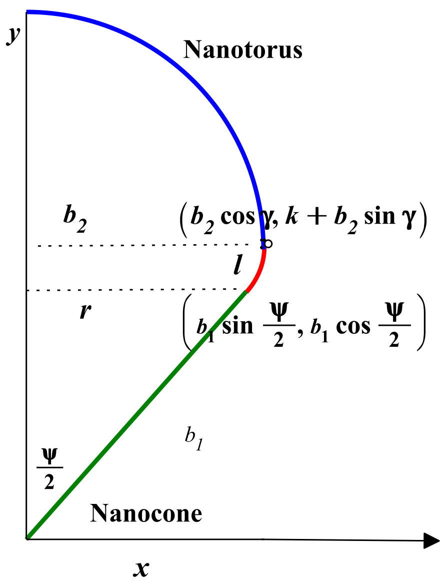

Fig. 5: Geometry of the joining curve between nanocone and nanotorus.

the $y-$axis. The curve that connect both structures has arc length l touches the nanostructures at $(b_1 \sin\psi/2, b_1 \cos\psi/2)$ to the cone where $b_1 = r\csc(\psi/2)$ and at $(b_2\cos\gamma, K + b_2 \sin\gamma)$ to torus as shown in Figure 5.
We discover that $y = y(x)$ denotes an element with arc length ds. The required curve that minimizes $J[y]$ has a particular definition:

$$J[y] = \int_0^l \kappa^2 ds + \lambda \int_0^l ds,$$

where κ denotes the axial curvature, and λ is a Lagrange multiplier related to the fixed length constraint. κ_2 is the rotational curvature and here it is assumed to be zero. Consequently, curvature may be defined as in [9] of the following definition:

$$\kappa = \pm\left(\lambda + \frac{\alpha}{(1+y'^2)^{\frac{1}{2}}}\right)^{\frac{1}{2}}, \qquad (5)$$

3 Results and Discussion

3.1 Hybrid production form on helicoid

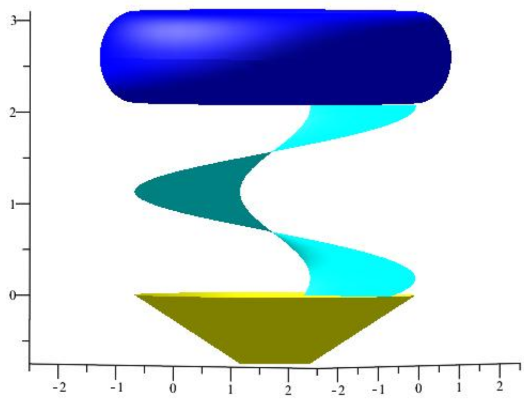

Fig. 6: Helicoid surface used as a smooth transition region between the nanocone and the nanotorus for values $r_c = 2$, $R_t = 2$ and $B = 2.6$.

In this section, we utilize the helicoid to vertically connect the nanocone on one side with the nanotorus on the other. The helicoid creates a local connection between certain nanocone and nanotorus boundary curves. Accordingly, it forms a smooth transition area instead of to a global boundary-to-boundary surface. We consider equation (2) to represent the helicoids surface in this scenario. For the cone-helicoid junction, the cones equation is provided in equation (3):

$$z = r\left(\frac{h_c}{r_c}\right). \tag{6}$$

At the point of (r_c, z_1), the helicoid starts at the same height of the cone with $r = r_c$, this gives

$$\frac{1}{A_1}\log(A_1 r_c) + A_2 = h_c,$$

which results

$$A_2 = h_c - \frac{\log(A_1 r_c)}{A_1}. \tag{7}$$

By matching the gradients, we obtain

$$\frac{h_c}{r_c} = \frac{1}{r_c},$$

this gives

$$h_c = 1. \tag{8}$$

For the helicoid-torus junction, the torus equation as given in equation (4) can be expressed as:

$$z = B + \sqrt{{R_t}^2 - r^2}, \tag{9}$$

where B is a constant indicated by the $z-$axis position of the torus. At the joining point (r_t, z_2) with $r = r_t$, for both structures the height must be the same, from (2) and (9) we obtain:

$$\frac{1}{A_1}\log(A_1 r_t) + A_2 = B + \sqrt{{R_t}^2 - {r_t}^2}. \tag{10}$$

After matching the gradients, we indicate:

$$\frac{1}{r_t} = \frac{-r_t}{\sqrt{{R_t}^2 - {r_t}^2}},$$

which gives:

$$r_t = \frac{R_t}{\sqrt{5}}. \tag{11}$$

By solving (10) numerically using (7), (8) and (11) with specific values for r_c, R_t and B we obtain values for A_1 and A_2 which determine the joining surface as in Figure 6. The helicoid offers a continuous transition between the nanocone and nanotorus along specific boundary curves, as observed in Figure 6. The smoothness and variational requirements C^1 continuity are met by this local junction. Furthermore, although not spanning the whole edge of either structure, it serves as a physically significant representation of nanoscale connections.

3.2 Hybrid production form on the calculus of variations

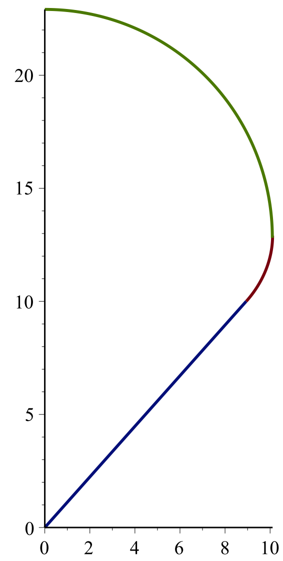

Fig. 7: 2D joining between nanocone and nanotorus with prescribed value $b_1 = b_2 = 10$, $\gamma = 0..\pi/2$, $l = 3.2$ and $\psi = 83.60$.

We are considering the positive case of (5), as long as the joint curvature continues to remain positive. Our substitution of $\tan\theta = y$ into (5) modifies it to align accordingly

$$\kappa_= (\lambda + \alpha\cos\theta)^{1/2}.$$

For the curvature, $\kappa = \frac{y''}{(1+y'^2)^{3/2}}$ and considering the first derivative of y, we may conclude

$$\frac{dy}{d\theta} = \frac{\sin\theta}{(\lambda + \alpha\cos\theta)^{1/2}},$$

and

$$\frac{dx}{d\theta} = \frac{\cos\theta}{(\lambda + \alpha\cos\theta)^{1/2}}.$$

Using a same calculations as in [25], and from the boundary condition (B. C) where y' changes from $y'(b_1\sin\psi/2) = -\tan\psi/2$ at the cone to $y'(b_2\cos\gamma) = -\cot\gamma$ at the torus, we obtain that

$$b_2\cos\gamma - b_1\sin\psi/2 = \beta\{2[E(\phi_1,k) - E(\phi_0,k)] - [F(\phi_1,k) - F(\phi_0,k)]\}, \tag{12}$$

$$y_0 = 2\beta k(\cos\phi_0 - \cos\phi_1) + b_1\cos\psi/2, \tag{13}$$

$F(\phi,k)$ and $E(\phi,k)$ indicate the first and second kinds of the standard Legendre incomplete elliptic integrals, correspondingly. Noting that $\phi_0 = \sin^{-1}(\sqrt{\frac{1-\sin\psi/2}{2k^2}})$ with

$\phi_1 = \sin^{-1}(1/\sqrt{2}k)$. From the arc length constraint equation:

$$l = \int_{b_1 \sin\psi/2}^{b_2 \cos\gamma} (1 + y'^2)^{1/2} dx,$$

now if we substitute $y' = \tan\theta$ to rewrite the following:

$$l = \beta[F(\phi_1, k), F(\phi_0, k)]. \tag{14}$$

Replacing (14) into (12) to have

$$\mu = 2\left(\frac{E(\phi_1, k) - E(\phi_0, k)}{F(\phi_1, k) - F(\phi_0, k)}\right) - 1, \tag{15}$$

with $\mu = (b_2 \cos\gamma - b_1 \sin\psi/2)/l$. As a result, if we assume specific values for b_1, b_2, γ, l and ψ, then we may solve (15) numerically to obtain k. Therefore (14) gives the value of β, this gives y_0 from (13), as demonstrated in Figure 7.

Here we state that this study produces hybrid nanoscale structure using curvature-depend models as in the literature. However, the novelty of our approach is emphasized by expanding the applicability for nanocone and nanotorus connections, which deals with more complex scenario because of the higher curvature gradients and conical geometry. Moreover, the proposed model in this study introduces the employing of helicoid surface which conforms the nanocone and nanotorus conjoining special needs that are the twisting and asymmetric curvature transitions which in contrast with other minimal surfaces. The special geometry of the helicoid leads to greater flexibility in dealing with challenging curvature, therefore enhances structural stability and continuity along the junction. We examined the impact of the proposed models on mechanical characteristics, particularly possible uses in nanofluidic devices and nanoelectromechanical systems. This comparative analysis confirms the originality of this study, especially in expanding mathematical modeling approaches for complicated nanostructure conjoining behind models depend on catenoid.

4 Conclusion

This study states the hybrid production process for constructing carbon nanostructure: nanocone and nanotorus. Identifying the critical connection area between the structures have been presented based on two techniques. First, calculating Euler-Lagrange equation by reducing the elastic energy. While the other way focus on reducing the Willmore energy using a minimal surface called a helicoid. During the both cases the continuous and smooth conjoining was expected. Thus, stable and efficient hybrid nanostructures configurations are produced.

Developed mechanical features have been shown by the hybrid nanocone-nanotorus structures. In particular, the new structures own a strong form and low scattering comparing with the original structures. The primary features of the carbon nanostructures were maintained during the connection process. As a result, our models have significant applications in nanoscale mechanics and fluidic process, while the properties of the original structure are reserved. Nevertheless, these encouraging outcomes, certain challenges require attention. This includes finding a specific parameter value that enables smooth transitions in complex structures and dealing with the computational limitations that occur through the modeling of large-scale structures.

Future research may focus on producing more hybrid configurations from other nanostructures. Also, different minimal surface can be used to generate new structures. On the other hand, including nonlocal components into the model can results in comprehensive understanding of the conjoining procedure, especially the interaction of molecular consideration.

Using advanced manufacturing methods as experimental verification may leads to enhancing the models credibility. Such as electron beam lithography and chemical vapor deposition which are very successful in complex cases. Further, other methods examine the integrity of the models as transmission electron microscopy and atomic force microscopy.

Moreover, new nanostructures advance mechanical stability and liquid transport efficiency according to their smooth curvature transitions. Thus, they might be used in nanofluidic devices and nanoelectromechanical systems. Moreover, computational simulations theories may support the experimental investigations by giving some explanations of the thermal, electronic, and mechanical features of these hybrid structures.

This integrated approach reducing the gap between theoretical perspective and the practical implications which leads to optimization possibilities for these new structures in manufacturing procedures in nanoscale.

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