Mechanics of tunable helices and geometric frustration in biomimetic seashells

Qiaohang Guo\textsuperscript{1,2,3(a)(b)}, Zi Chen\textsuperscript{3(a)(c)}, Wei Li\textsuperscript{1,4}, Pingqiang Dai\textsuperscript{1,4}, Kun Ren\textsuperscript{4}, Junjie Lin\textsuperscript{4}, Larry A. Taber\textsuperscript{3} and Wenzhe Chen\textsuperscript{1,4}

\textsuperscript{1} College of Materials Science and Engineering, Fuzhou University - Fujian 350118 China
\textsuperscript{2} Department of Mathematics and Physics, Fujian University of Technology - Fujian 350118 China
\textsuperscript{3} Department of Biomedical Engineering, Washington University in St. Louis - St. Louis, MO 63130, USA
\textsuperscript{4} College of Materials Science and Engineering, Fujian University of Technology - Fujian 350118 China

received 17 October 2013; accepted in final form 13 March 2014
published online 28 March 2014
PACS 46.25.-y – Static elasticity

Abstract – Helical structures are ubiquitous in nature and engineering, ranging from DNA molecules to plant tendrils, from sea snail shells to nanoribbons. While the helical shapes in natural and engineered systems often exhibit nearly uniform radius and pitch, helical shell structures with changing radius and pitch, such as seashells and some plant tendrils, add to the variety of this family of aesthetic beauty. Here we develop a comprehensive theoretical framework for tunable helical morphologies, and report the first biomimetic seashell-like structure resulting from mechanics of geometric frustration. In previous studies, the total potential energy is everywhere minimized when the system achieves equilibrium. In this work, however, the local energy minimization cannot be realized because of the geometric incompatibility, and hence the whole system deforms into a shape with a global energy minimum whereby the energy in each segment may not necessarily be locally optimized. This novel approach can be applied to develop materials and devices of tunable geometries with a range of applications in nano/biotechnology.

Introduction. – Helical structures are basic building blocks in biological and engineering systems, such as DNA \cite{1,2}, plant tendrils \cite{3–5}, seashells \cite{6,7}, curly hair \cite{8}, cholesterol molecules \cite{9}, and nanoribbons \cite{10,11}. Recent work has shown that helical ribbon morphology can be controlled by the mechanical balance between surface stresses or internal residual strains and the induced elastic stretching and bending \cite{5,12–16}. Importantly, the generation of helical morphology requires both mechanical anisotropy, such as anisotropy in surface stress \cite{17}, residual strain, elastic properties \cite{18}), and geometric mis-orientation between the principal mechanical axes and geometric axes (length, width, thickness) of the structure.

However, many of the helical structures studied with theoretical and experimental approaches exhibit uniform radius and pitch \cite{12,13,17–19}. Helical morphologies of variable radius, pitch and width are less heavily investigated. As typical representatives of helical shapes with geometric parameters, seashells have long fascinated scientists with their aesthetic beauty that roots in their self-similar, spiraling shapes with left-right asymmetry. Moseley first modeled the geometry of the coiling molluscan shell as a logarithmic spiral \cite{20}. Afterwards, a number of theoretical models of molluscan shells have been developed on the geometric properties of shell growth and morphogenesis \cite{21–23}. In recent years, some theoretical models have addressed the biological processes taking place at the growing edge and the growth kinematics of shell aperture \cite{6,7,24–28}. While the morphogenesis of seashells is not the main focus of the current study, it is of interest, from an engineering point of view, to develop both theoretical and experimental strategies of designing shapes inspired by nature, \textit{e.g.}, structures that mimics the seashells. In this letter, we first develop a theoretical framework for helical morphologies with tunable geometric parameters such as principal radii of curvature, width and helix angle, but without self-contact. Then we address the mechanics of geometric frustration due to self-avoidance restriction, and report the generation of three-dimensional helical morphologies where the energy

\textsuperscript{(a)}Contributed equally to this work.
\textsuperscript{(b)}E-mail: guoqh@fjut.edu.cn
\textsuperscript{(c)}E-mail: chen.z@seas.wustl.edu
minimization is achieved on a global scale but not locally. According to this principle, we designed a helical, seashell-like structure through table-top experiments. This study can promote the understanding of morphogenesis in biological systems [13], and inspire new design principles for novel materials and devices of tunable morphologies or structures that can change configurations in response to external stimuli [29], with applications in nanofabrication [10,18,30] and bio-inspired technology [31,32].

**Theoretical model.** — In this work, the ribbon is considered as an elastic sheet with length $L$, width $w(s)$, and thickness $H \ll w$. The ribbon thus features rectangular cross-sections with changing width, and the principal geometric axes are along the length ($d_x$), width ($d_y$), and thickness ($d_z$) directions, which form an orthonormal triad, $\{d_x, d_y, d_z\}$, that convolutes with the bent and twisted ribbon in three-dimensional space.

Chen et al.’s recent works [12] have shown that the equilibrium configuration can be determined by both local and global energy minimization when the deformed ribbon has constant principal curvatures, and does not have any self-contact. Here, we first deal with the more general case of bi-axial bending with varying principal curvatures along the centerline, also without self-contact. In this case, the ribbon will have principle curvatures $\kappa_1(s)$ and $\kappa_2(s)$ along the directors $d_1 = \cos \phi d_x - \sin \phi d_y$ and $d_2 = \sin \phi d_x + \cos \phi d_y$ oriented at an angle $\phi$ relative to $d_z$ within the plane of the ribbon (see fig. 1). In the global cartesian coordinate system, the coordinates of a point $P(s)$ (parameterized by the arclength $s$) on the centerline can be obtained by integrating the following equations [14]:

$$\frac{dP}{ds} = \cos \phi r_1 + \sin \phi r_2,$$

$$\frac{dN}{ds} = \kappa_1(s) \cos \phi r_1 + \kappa_2(s) \sin \phi r_2,$$

$$\frac{dr_1}{ds} = -N \kappa_1(s) \cos \phi,$$

$$\frac{dr_2}{ds} = -N \kappa_2(s) \sin \phi,$$

where $N = d_z \equiv d_x \times d_y = r_1 \times r_2$ is unit normal to the ribbon, together with the boundary conditions $P(0) = X(0) E_x + Y(0) E_y + Z(0) E_z$, $N(0) = E_z$, $r_1(0) = \cos \phi E_x - \sin \phi E_y$ and $r_2(0) = \sin \phi E_x + \cos \phi E_y$. It is worth noting that although analytic expressions can be obtained when $\kappa_1(s)$ and $\kappa_2(s)$ are both constant [12,14], in the more general case of interest where $\kappa_1(s)$ and $\kappa_2(s)$ have an arclength dependence, the coordinates of the centerline can be solved numerically.

In the presence of bi-axial bending curvatures, the deformed ribbon exhibit strain components $\epsilon_{xx}$, $\epsilon_{yy}$, $\epsilon_{xy}$, and $\epsilon_{zz}$, which are considered uniform throughout the $d_y$ direction of the ribbon (when geometric nonlinearity is relatively weak). More general consideration involving geometric nonlinearity can be done following the recent work of Chen et al. [33]. Here, we choose not to include the nonlinear geometric effects for the clarity of statement about the procedure. By superposition we obtain the strain tensor $\gamma = \gamma_{ij} d_i \otimes d_j (i, j \in \{x, y, z\})$ with components

$$\gamma_{xx} = \epsilon_{xx} + z(\kappa_1 \cos^2 \phi + \kappa_2 \sin^2 \phi) + \gamma_{0xx}(z),$$

$$\gamma_{xy} = \epsilon_{xy} + z(\kappa_1 - \kappa_2) \sin \phi \cos \phi + \gamma_{0xy}(z),$$

$$\gamma_{yy} = \epsilon_{yy} + z(\kappa_1 \sin^2 \phi + \kappa_2 \cos^2 \phi) + \gamma_{0yy}(z),$$

$$\gamma_{zz} = \epsilon_{zz} + z(k_3 + \gamma_{0zz}(z)).$$

Here, $z \in [-H/2, H/2]$ is the distance of any point in the ribbon away from the midplane, while $\gamma_{0ij}(z)$ represents the residual strain component within the initially flat ribbon.

On the top and bottom surfaces ($z = \pm H/2$), effective surface stress $f^\pm$ serve as the driving forces for spontaneous deformation. The potential energy per unit area in the ribbon is $\Pi = f^- : \gamma|_{z=-H/2} + f^+ : \gamma|_{z=H/2} + \int_{-H/2}^{H/2} \gamma : C : \gamma dz$, where $C$ denotes the fourth-order elastic constant tensor. The equilibrium configuration can be achieved by minimizing the potential energy $\Pi : \partial \Pi / \partial \gamma = 0$, where $\gamma$ represents any of the undetermined parameters [12].

Next, we consider the more interesting scenario with potential self-contact [19]. For example, for an intrinsically helical ribbon with a linearly varying width, $W = W_0 - \alpha s$ (or constant, i.e., $\alpha = 0$), where the minimal energy shape cannot be achieved due to the potential self-contact restriction (here we use the term “geometric frustration” to describe this situation), what will the possible equilibrium configuration be? Here we note
that the geometric frustration discussed in this work is different from the “geometrical frustration” discussed by Armon et al. [13,34] that mainly concerns the competition between bending and stretching energy of an elastic strip. Of course, when there is no self-contact, the system achieves both local and global energy minimization. More specifically, given a virtually equilibrium configuration with natural principal curvatures in the forbidden regime (i.e., with self-penetration), what will be the actual minimum-energy configuration be? In a pioneering work, Chouaieb and co-workers [19] studied the specific case for the self-contacting case of a uniform helical rod. Here, the geometry and mechanics involved are more complicated, since the ribbon can have a varying width, and non-constant principal curvatures. We first do local energy minimization to find the equilibrium shape without considering self-avoidance, i.e., when there is no energy penalty for doubly occupying the same space. For a segment of more than one complete turn, however, self-contact becomes inevitable when the projected distance (along the helix axis direction) between adjacent turns are smaller than the pitch, i.e.,

\[ R \left( \sin \left( \frac{W_1}{2R \sin \theta} \right) + \sin \left( \frac{W_2}{2R \sin \theta} \right) \right) \leq D, \] (6)

where \( D = 2\pi(k_1 - k_2)\sin \phi \cos \phi/(k_1^2 \cos^2 \phi + k_2^2 \sin^2 \phi) \) is the pitch, \( R = 1/[k_1^2 \cos(\phi + \theta) + k_2^2 \sin(\phi + \theta)] \) is the radius of curvature along the helix axis direction (see fig. 2), and \( \theta = \arctan[(k_1 - k_2) \cos \phi \sin \phi/(k_1^2 \cos \phi + k_2^2 \sin \phi)] \) is the angle between the helix axis and the longitudinal axis of the ribbon. When the radii of curvature along the ribbon are such that the self-contact happens everywhere, a tightly coiled ribbon results. This is similar to, but more complicated than, the example of a stress-free helical rod that cannot achieve its equilibrium configuration due to self-avoidance constraint [19]. The strain-energy function for a hyperelastic ribbon is \( W_{\text{tot}} = \int W(\gamma - \gamma^*) \, dr = \int \frac{1}{2}(\gamma - \gamma^*) \cdot K(\gamma - \gamma^*) \, dr \), where \( \gamma^* \) are the strains in the unstressed reference configuration where there are no resultant moments everywhere, \( \mathbf{r} \) is the vector of a point in the ribbon, and \( K \) is a 3-by-3 symmetric positive-definite matrix [19]. The minimum-energy configuration can be found by first constructing the energy level sets and then tracing the tangential points between the energy level set and the inaccessible (forbidden) region due to self-penetration. In principle, there are two tangential points, indicating two possible solutions (local minima) with opposite handedness. In reality, however, the configuration with smaller energy will be the global equilibrium featuring a preferred handedness.

**Biomimetic seashell structure through table-top experiments.** – As a proof of concept, we designed table-top experiments to manufacture biomimetic seashells (Turritella). Turritella is a common kind of dextral seashell species, and the typical surface of the shell is shown in fig. 3(a). The radius and width of the seashell are constantly changing, and the adjacent turns are in contact. We made markers on the centerline of the seashell and used a Panasonic HD digital camera (DMC-FZ100) to obtain digital images both from top and front to get the three-dimensional information. The images were subsequently analyzed using custom-made image analysis algorithms developed in Matlab. We develop a strategy to mathematically model the spatial configuration of the
centerline of a seashell structure. Ideally, the centerline of the seashell lies on the surface of a cone (see fig. 3(b), (c)). The cone angle ($\alpha$), the helix angle ($\theta$), the length of the centerline ($L$), were measured to be 16.6°, 12° and 36 cm, respectively. The radius of the intrinsically helical turn changes almost linearly from 1.3 cm to 0.1 cm.

Considering the feature of the seashell surface, we designed a table-top experiment so as to set up an energy hypothesis of biomimetic seashell structure. In our experiments, one sheet of latex rubber (thickness $H_1$) was pre-stretched bi-axially and bonded to two layers. One was an unstrained elastic strip of thick, pressure-sensitive adhesive (thickness $H_2$), and the other was a piece of un-stretched thin latex rubber sheet along a mis-orientation angle $\phi$ with respect to the principal axes (see the methods in [12,33]). Thus, the total thickness of the bonded strip is $H = 2H_1 + H_2$. If there are no overlap and also the same strain in segments, the local morphology can be predicted [12,33]). So, the pre-strain along the $d_y$ direction, $q$, was 0.3, while the pre-strain along the horizontal direction, $p$, changed from 0.25 to 0.90 in a piecewise uniform manner and the corresponding lengths of the segments before stretching are shown in fig. 4.

Upon release, the bonded composite sheet deformed into seashell-like shapes (see fig. 5(a)). If the adjacent turns were allowed to overlap without additional energy cost, the configurations of each segment would have conformed to those shown in fig. 5(b). It is noteworthy that all the segments would come into self-contact if the condition in eq. (6) is satisfied, and that the chirality would change from right-handed to left-handed. This change of chirality can be naturally interpreted using the recently developed elasticity model [12], whereby the handedness is given by the sign of the helix angle, $\Phi = \arctan(\kappa_1 - \kappa_2) \sin \phi \cos \phi / (\kappa_1 \cos^2 \phi + \kappa_2 \sin^2 \phi)$. When the first principal curvature is smaller than the second, the helical ribbon is left-handed (the bottom segment in fig. 5(b)); while the first principal curvature becomes smaller than the second, the helical shape becomes right-handed (the top five segments in fig. 5(b)); a ring-like shape results when the two principal curvatures are equal (the second last segment in fig. 5(b)). But since self-penetration will lead to an infinite energy penalty, and hence not allowed, the overall geometric compatibility requires that the ribbon conform to a seashell-like shape as shown in fig. 5(a), featuring a right-handed, tightly coiled configuration, consistent with the theoretical prediction (the predominant handedness in the unstressed configuration prevails). And the simulated centerline from the mimetic seashell is shown in fig. 5(c).

However, the cone angle of the mimetic seashell measured is $\alpha = 11.2°$, which is smaller than the real seashell. It is possible to change the experimental parameters so that the change in radii goes faster, if the increase of pre-stretch values along the ribbon becomes sharper. There is, however, a limit as for how much the material can be pre-stretched while not undergoing plastic deformation (for the latex rubber that we used, we observed empirically that the pre-stretch cannot go beyond 1, otherwise plastic deformation is inevitable).

Moreover, we show that our computational model can be employed to assist in the design of versatile helical/multistable structures through strain engineering [35,36]. For example, fig. 6(a) shows the large deformation of a strained bilayer strip with self-contact using Consol Multiphysics 4.3a. The methodology is detailed in recent works [35,36]. However, numerical convergent issues are currently preventing us from fully simulating...
the biomimetic seashell structure presented in this work. On the other hand, when the geometry constraint has no effect, the coiled shape does have a co-existing left- and right-handed segments. For example, fig. 6(b) shows the co-existence of left- and right-handed helical segments when the pre-stretches are relatively small (1/25 of the actual pre-stretches) so that there is no self-contact.

Conclusions. – We develop a comprehensive theoretical framework for spontaneous helical ribbon structures with tunable geometric parameters and no self-contact by employing continuum elasticity, differential geometry, and stationary principles. Moreover, for ribbons that cannot access the locally stable shapes due to self-penetration, we show that a tightly coiled helical shape can result with a preferred handedness so that the total energy is globally minimized but not locally. Based on this principle, we designed a helical, seashell-like structure through simple table-top experiments. This study represents a new paradigm for predicting and prescribing helical structures, and can inspire new design principles for novel materials and devices of tunable morphologies with broad applications in biological and engineering practises.

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The authors would like to thank YUSHAN HUANG, ZHEN LIU, SI CHEN for their assistance in the experiments and the anonymous reviewers for their valuable comments and feedbacks. This work has been in part supported by the National Natural Science Foundation of China (Grant No. 11102040), Projects of International Cooperation and Exchanges NSFC (Grant No. 11201001044), Foundation of Fujian Educational Committee (Grant No. JA12238), the Sigma Xi Grants-in-aid of Research (GIAR) program, the American Academy of Mechanics Founder’s Award from the Robert M. and Mary Haythornthwaite Foundation, and the Society in Science, The Branco Weiss Fellowship, administered by ETH Zürich (ZC).

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