Electronic Supplementary Material (ESI) for Nanoscale

Electronic Supplementary Information (ESI)

Long-range Linear Elasticity and Mechanical Instability of Self-scrolling Binormal Nanohelices under Uniaxial Load

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A Cosserat curve, i.e., a directed curve with an orthonormal triad of directors and specified by four vector fields, follows the basic equilibrium equations [1]:

$$\hat{\tau}_\alpha - \varepsilon_{\alpha\beta\gamma}\tau_\beta W_\gamma = 0, \tag{S1a}$$

$$\hat{m}_\alpha - \varepsilon_{\alpha\beta\gamma}\left(m_\beta W_\gamma + \tau_\beta y_\gamma\right) = 0 \tag{S1b}$$

where τ and m are the total force and torque across the cross section of the curve, respectively; ε is the permutation tensor, W and y are the director and position deformation measures, respectively. The Greek subscripts α, β, γ take on the values 1, 2, 3. $\hat{()} = \partial/\partial S = \lambda \dot{()} = \lambda\,\partial/\partial s$, and $\lambda = \partial s/\partial S$ is the stretch of the curve with S the arc length along a fixed reference configuration and s the one along a deformed configuration [2, 3].

As presented in Figure 2(e-f) of the paper, two types of helices with a rectangular cross section are considered, they are named normal and binormal helices, respectively [4, 5]. Assuming that a helix H_I with the radius a_0, pitch b_0, length l_0 and number of turns N is curled from a nanobelt with a width of w and a thickness of t ($w > t$), when a tensile force F is exerted along the helical axis, the helix is elongated with a length of L and it is deformed to a new helical shape H_F, i.e. a radius a, a pitch b and a length l, simultaneously. Therefore, in the model H_I is the fixed reference configuration and H_F is the deformed one, whose director basis $\boldsymbol{D}_i$ (i=1,2,3) and $\boldsymbol{d}_i$ are defined by a set of Euler angles ϕ_0, θ_0, ψ_0 and ϕ, θ, ψ, respectively. For the configuration of helix, ϕ_0, θ_0, $\dot{\psi}_0$, ϕ, θ, $\hat{\psi}$ are all constants [6]. We choose the third director $\boldsymbol{D}_3$ of H_I along the tangent to the centerline of the helical ribbon axis, and the force F along the $\boldsymbol{e}_3$ axis of the fixed Cartesian basis. $\boldsymbol{D}_1$, $\boldsymbol{D}_2$ and $\boldsymbol{d}_1$, $\boldsymbol{d}_2$ are assumed to be along the direction of the largest and smallest bending stiffness of the cross section in H_I and H_F, respectively.

The director deformation measures $W^{(0)}$ of H_I for a normal and a binormal helix are given by

$$W_{1N}^{(0)} = -\dot{\psi}_0 \sin\theta_0,\; W_{2N}^{(0)} = 0,\; W_{3N}^{(0)} = \dot{\psi}_0 \cos\theta_0. \tag{S2a}$$

$$W_{1B}^{(0)} = 0\,,\; W_{2B}^{(0)} = \dot{\psi}_0 \sin\theta_0\,,\; W_{3B}^{(0)} = \dot{\psi}_0 \cos\theta_0\,. \tag{S2b}$$

respectively. We use W, director deformation measures for H_F, in the equilibrium equation Eq. (S1b) and obtain:

$$(A-C)W_{1N}W_{3N} - AW_{1N}^{(0)}W_{3N} + CW_{3N}^{(0)}W_{1N} + (E_1 - E_3)y_{1N}y_{3N} + E_3 y_{1N} = 0\,, \tag{S3a}$$

$$W_{2N}\left[-A\left(W_{1N} - W_{1N}^{(0)}\right) + BW_{1N}\right] = 0\,, \tag{S3b}$$

for a normal helix, and

$$(B-C)W_{2B}W_{3B} - BW_{2B}^{(0)}W_{3B} + CW_{3B}^{(0)}W_{2B} + (E_2 - E_3)y_{2B}y_{3B} + E_3 y_{2B} = 0\,, \tag{S4a}$$

$$W_{1B}\left[-AW_{2B} + B\left(W_{2B} - W_{2B}^{(0)}\right)\right] = 0\,, \tag{S4b}$$

for a binormal helix, where E_1=E_2=$KGtw$, E_3=Etw, A=EI_1, B=EI_2, and $C = 4GI_1I_2/(I_1+I_2)$ according to the scaled torsional stiffness [7]. K is the Timoshenko shear coefficient which is related to the Poisson's ratio v through $K = (5+5v)/(6+5v)$ [8]. E and G=E/2(1+v) are the Young's and shear moduli of the nanobelt, respectively. I_1= $w^3t/12$ and I_2= $wt^3/12$ are the moment of inertia.

Since the shape of H_F is determined by the applied force, Eqs. (S3b) and (S4b) indicate that for a helical solution, the director deformation measures W have the form of:

$$W_{1N} = -\hat{\psi}\sin\theta\,,\; W_{2N} = 0\,,\; W_{3N} = \hat{\psi}\cos\theta \tag{S5a}$$

for a normal helix, and

$$W_{1B} = 0\,,\; W_{2B} = \hat{\psi}\sin\theta\,,\; W_3 = \hat{\psi}\cos\theta \tag{S5b}$$

for a binormal helix. The relation $\hat{\psi} = \dot{\psi}_0$ is derived from $\hat{\psi} = \lambda/\sqrt{a^2+b^2}$ [1]. The position vectors obtained from Eq. (1a) of H_F are expressed by:

$$y_{1N} = -\frac{F}{E_1}\sin\theta\,, y_{2N} = 0\,,\; y_{3N} = \frac{F}{E_3}\cos\theta + 1\,, \tag{S6a}$$

for a normal helix; and

$$y_{1B} = 0\,, y_{2B} = \frac{F}{E_2}\sin\theta\,,\; y_{3B} = \frac{F}{E_3}\cos\theta + 1\,, \tag{S6b}$$

for a binormal helix. From Eq. (S6), the stretch λ is obtained by:

$$\lambda = \sqrt{\frac{F^2}{E_1^2}\sin^2\theta + \left(\frac{F}{E_3}\cos\theta + 1\right)^2}\,, \tag{S7}$$

as well as the radius and pitch of H_I and H_F in terms of the Euler angles for both normal and binormal helices :

$$a_0 = \frac{\sin\theta_0}{\dot{\psi}_0},\; b_0 = \frac{2\pi\cos\theta_0}{\dot{\psi}_0}, \tag{S8a}$$

$$a = \frac{1}{\dot{\psi}_0}\left[\left(\frac{F}{E_3}\cos\theta + 1\right) - \frac{F}{E_1}\cos\theta\right]\sin\theta\,, b = \frac{2\pi}{\dot{\psi}_0}\left[\frac{F}{E_1}\sin^2\theta + \left(\frac{F}{E_3}\cos\theta + 1\right)\cos\theta\right] \tag{S8b}$$

By combination of Eq. (6) and the result of $W_\alpha^{(0)}$, W_α, $\dot{\psi} = \dot{\psi}_0$, Eq. (3a) and (4a) are given by:

$$\left(\frac{1}{E_3} - \frac{1}{E_1}\right)\cos\theta\sin\theta F^2 + \sin\theta F - C\dot{\psi}_0^2(\cos\theta - \cos\theta_0)\sin\theta$$
$$+ EI_1[1-(\Delta-1)\delta_{i2}]\dot{\psi}_0^2(\sin\theta - \sin\theta_0)\cos\theta = 0 \tag{S9}$$

where $\Delta \equiv I_2/I_1$, $i = 1$ (or $i = 2$) for a normal (or binormal) helix and δ_{i2} is the Kronecker delta.

Furthermore, the torque (M) along the same direction as that of the force F is expressed by:

$$M = EI_1[1-(\Delta-1)\delta_{i2}]\dot{\psi}_0(\sin\theta - \sin\theta_0)\sin\theta + C\dot{\psi}_0(\cos\theta - \cos\theta_0)\cos\theta \tag{S10}$$

The spring constant k of H_F is deduced from Eqs. (S8) and (S9) according to the Hooke's law *k=dF/dL:*

$$k = -\frac{P_1 P_4}{N(P_3 P_4 + P_2)},$$

where $P_1 \equiv \left[\dot{\psi}/2\pi\right] \Big/ \left[1 + 2F\cos\theta\left(\frac{1}{E_3} - \frac{1}{E_1}\right)\right]$,

$$P_2 \equiv 2\left(\frac{1}{E_3}-\frac{1}{E_1}\right)\cos\theta\sin\theta F+\sin\theta\,,$$

$$P_3 \equiv -\left[\frac{1}{E_1}+\left(\frac{1}{E_3}-\frac{1}{E_1}\right)\cos^2\theta\right]\Big/\left[1+2F\cos\theta\left(\frac{1}{E_3}-\frac{1}{E_1}\right)\right],$$

$$P_4 \equiv \left(\frac{1}{E_3}-\frac{1}{E_1}\right)\frac{1-2\cos^2\theta}{\sin\theta}F^2-\frac{\cos\theta}{\sin\theta}F+\dot{\psi}_0^2\{EI_1[1-(\Delta-1)\delta_{i2}]-C\}\frac{1-2\cos^2\theta}{\sin\theta}$$
$$-EI_1[1-(\Delta-1)\delta_{i2}]\dot{\psi}_0^2\sin\theta-C\dot{\psi}_0^2\cos\theta_0\frac{\cos\theta}{\sin\theta}$$

(S11)

By measuring the geometry parameters a_0, b_0, t, w, N of the helix H_I in its initial shape and the applied force F or torque M, Eqs. (S7-S11) can be used to calculate the radius a, pitch b, and the spring constant k of H_F with the conservation of length $l=\lambda l_0$, where $l_0 = N\sqrt{(2\pi a_0)^2+b_0^2}$ and $l = N\sqrt{(2\pi a)^2+b^2}$ are the unwound length of the nanobelt after and before loading, respectively. We note that the shear deformation and extension have been taken into account in the Cosserat curve model.

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Nomenclature

τ(N): the total force across the cross section of the curve.

m(N m): the total torque across the cross section of the curve.

ε: permutation tensor.

W: director deformation measures.

y(m): position deformation measures.

α, β, γ: Greek subscripts.

S(m): arc length along a fixed reference configuration.

s(m): arc length along a deformed configuration.

λ: stretch of the curve.

H_I: helix before loading.

a_0(m): radius of helix H_I.

b_0(m): pitch of helix H_I.

l_0(m): length of helix H_I.

N: number of turns of helix.

w(m): width of nanobelt.

t(m): thickness of nanobelt.

F(N): loading force along the helical axis.

H_F: helix after loading.

L(m): elongated length of helix.

a(m): radius of helix H_F.

b(m): pitch of helix H_F.

l(m): length of helix H_F.

$\mathbf{D}_i$(i=1,2,3): director basis of helix H_I along three orthonormal basis of fixed rectangular Cartesian coordinate system.

$\mathbf{d}_i$(i=1,2,3): director basis of helix H_I along three orthonormal basis of fixed rectangular Cartesian coordinate system.

ϕ_0, θ_0, ψ_0(rad): set of Euler angles defining director basis $\boldsymbol{D}_i$.

ϕ, θ, ψ(rad): set of Euler angles defining director basis $\boldsymbol{d}_i$.

$W_{iN}^{(0)}$, $W_{iB}^{(0)}$ (i=1,2,3): director deformation measures of H_I along three orthonormal basis of fixed rectangular Cartesian coordinate system for a normal helix and a binormal helix, respectively.

W_{iN}, W_{iB} (i=1,2,3): director deformation measures of H_F along three orthonormal basis of fixed rectangular Cartesian coordinate system for a normal helix and a binormal helix, respectively.

E_i, A, B, C, P_j (i=1,2,3; j=1,2,3,4): Intermediate parameters.

E(Pa): Young's modulus of the nanobelt.

G(Pa): shear modulus of the nanobelt.

v: Poisson's ratio.

I_1, I_2(m^4): moment of inertia.

y_{iN}, y_{iB} (i=1,2,3)(m): position deformation measures of H_F along three orthonormal basis of fixed rectangular Cartesian coordinate system for a normal helix and a binormal helix, respectively.

δ_{i2} : Kronecker delta.

M(N m): torque along the helical axis.

k(N/m): spring constant of H_F.

v_{SiGe}: Poisson's ratio of SiGe.

v_{Si}: Poisson's ratio of Si.

v_{Cr}: Poisson's ratio of Cr.

x(m): distance between two adjacent exposed edges of the nanobelt along its width direction.

ΔL_S(m): relative stretch of nanobelt.

F_{cr} (N): critical compressive load causing buckling.

l_{cr} (m): critical length of helix before buckling.

Δ_{cr} (m): critical decrease of length of helix before buckling.

ξ (rad): pitch angle.

α_0 (N m^2): bending rigidity of the nanohelix.

s_0 (m): length of nanobelt.