International Journal of Solids and Structures 50 (2013) 3922–3933

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

A structural gradient theory of torsion, the effects of pretwist, and the tension of pre-twisted DNA

A.E. Giannakopoulos [a,*], N. Aravas [b,c], A. Papageorgopoulou [a], I. Vardoulakis [d]

[a] Department of Civil Engineering, University of Thessaly, 38334 Volos, Greece
[b] Department of Mechanical Engineering, University of Thessaly, 38334 Volos, Greece
[c] International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka 819-0395, Japan
[d] Faculty of Applied Mechanics and Physics, National Technical University of Athens, 15773 Athens, Greece

ARTICLE INFO

Article history:
Received 20 April 2013
Received in revised form 13 July 2013
Available online 11 August 2013

Keywords:
Gradient elasticity
Torsion
Pretwist
Size effect
DNA

ABSTRACT

A structural gradient theory of torsion of thin-walled beams is developed. A non-local estimate of the mean value of the angle of twist of the beam leads to a shear gradient that is energetically consistent with a bi-moment, in the spirit of the averaging theory of Vardoulakis and Giannakopoulos (2006). The geometric details of the cross section play the role of the microstructure of the beam, introducing a size effect in the torsion problem. The appropriate boundary conditions are derived from the variational formulation of the problem. The proposed gradient elasticity theory is identical to Vlasov's torsion theory of thin walled elastic beams. The tension of pre-twisted DNA is analyzed at high axial loads, where enthalpic elasticity prevails. A size effect is naturally introduced, indicating that shorter DNA lengths lead to stiffer response in torsion. It is shown also that the complete unwinding of DNA triggers the debonding of its strands.

1. Introduction

The averaging theories of Mechanics are based usually on the so-called simple theories, where local field variables are identified with mean values and the corresponding continua are described as locally homogeneous. However, when the field variables are locally not adequately represented by linear functions, the averaging procedures must be corrected to incorporate at least the effect of the local curvature and the resulting field theories are called higher gradient theories (Green and Rivlin, 1964). Vardoulakis and Giannakopoulos (2006) demonstrated these ideas by revisiting the engineering beam-bending theory. The idea of relating classical advanced theories of structures, like Timoshenko beams and Reissner–Mindlin plates (with rotary inertia and shear corrections), has also been used by Papargyri-Beskou et al. (2009) and showed equivalence with their corresponding reduced theories, like Bernoulli–Euler beams and Kirchhoff plates, but in their gradient elasticity formulation. Theory of ropes and cables (e.g. Costello, 1983) can also benefit from the present approach.

In the present work, we extend these ideas to the beam-torsion theory and model the deformation of pretwisted DNA molecules, employing the simplest version of Toupin–Mindlin gradient theory that involves an isotropic linear response and only one material constant additional to the standard elastic constants (Toupin, 1962 and Mindlin, 1964). This theory can be viewed as a first order extension of the classical elasticity theory, which assumes a strain energy density function that depends on the strains and the strain gradients (Georgiadis et al., 2004 and Georgiadis and Anagnostou, 2008). As will become more evident later-on in this work, the fore mentioned gradient elasticity theories involve complicate boundary conditions (Bleustein, 1967) and allow for boundary layer effects that can capture phenomena related to fracture (e.g. Georgiadis, 2003 and Shi et al., 2000), dislocations (e.g. Lazar and Maugin, 2005), dispersion phenomena at high frequencies (e.g. Vardoulakis and Georgiadis, 1997 and Papargyri-Beskou et al., 2009), to mention but few.

The classical linear elasticity theory of torsion of beams is based on the notion that the rotation (angle of twist) ϕ of the cross section varies linearly along a straight beam, and the strain energy per unit length of the beam $\bar{U}$ depends on the constant gradient (or "rate") of twist $\alpha = \frac{d\phi}{dz}$, where z is the coordinate along the beam axis (Sokolnikoff, 1956). The corresponding "structural constitutive equation" is of the form

$$T = \frac{\partial \bar{U}(\alpha)}{\partial \alpha} = GJ\alpha, \tag{1}$$

where T is the applied torque, G the elastic shear modulus, and J the torsional constant of the cross section.

* Corresponding author. Tel.: +30 24210 74179.
E-mail address: agiannak@uth.gr (A.E. Giannakopoulos).

0020-7683/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijsolstr.2013.08.003

Beams constitute parts of structural systems and are often loaded by axial forces and bending moments, in addition to torsion moments. Beams are often connected in ways that coupling phenomena between torsion, bending and stretching take place at their ends. A notable coupling case is the torsion-bending type of buckling (Timoshenko and Gere, 1961). Solving such problems can be very difficult in general.

In the present work we address the problem of *inhomogeneous* torsion and assume that the gradient of twist is not constant along the beam. We formulate a "gradient" (multipolar) linear elasticity theory for beam torsion and bring in the DNA's microstructure.

The new structural theory could be viewed as a "composite" averaging where non-affine "strains" are introduced as boundary conditions to the "representative volume element", which in this case is the cross section of the beam. Put in other words, this procedure is an averaging methodology that uses non- affine strain distributions as proposed originally by Mindlin (1964). In order to establish well-posed boundary value problems, the new higher-order theory requires the introduction of a new structural variable, the "bimoment"B, which was first introduced by Vlasov (1969) in his theory of thin-walled beams with open cross sections. This, in turn, introduces additional natural boundary conditions at the ends of the beam. The strain energy density per unit length of the beam $\bar{U}$ depends now not only on the rate of twist $\alpha = \frac{d\phi}{dz}$ but on its gradient $\bar{\bar{\kappa}} = \frac{d^2\phi}{dz^2}$ as well. The corresponding structural constitutive equations now become

$$T^{SV} = \frac{\partial \bar{U}(\alpha, \bar{\bar{\kappa}})}{\partial \alpha} = GJ\alpha \text{ and } B(\bar{\bar{\kappa}}) = \frac{\partial \bar{U}(\alpha, \bar{\bar{\kappa}})}{\partial \bar{\bar{\kappa}}} = \ell^2 GJ\bar{\bar{\kappa}} \quad (2)$$

where T^{SV} is the classical Saint–Venant torque and ℓ is a "structural length". In this approach, "size effects" become evident, since the additional constitutive Eq. (2b) introduces a length scale that unifies the elastic energy contributions from both the classical moment and the bimoment.

We apply the theory to the tension of a single DNA molecule that has been initially stretched by a high tensile load. DNA is a polymer of desoxyribonucleic acid, with high molecular weight (10^6–10^8), which resembles a double helix (Watson–Crick helix) of diameter 2 nm. It has a natural rate of twist of about 1.85 rad/nm (Bao, 2002). The main backbones of the helix are two parallel strands of phosphate sugar groups with an ester linkage, tying each one to the next sugar group all the way along the backbone. At right angles to the backbone are the bases, which are characteristic organic components of a nucleic acid molecule. They are held together in the middle by hydrogen bonds, making the DNA a compact and fairly rigid structure. A double-helical DNA chain has ten base pairs per helical turn of length 3.4 nm (Bao, 2002). Many viruses contain a DNA and can cause diseases that afflict humans, plants, and animals. The DNA of a virus must have enough torsional stiffness and strength to be able to drill through the tough bacterial cell walls. The DNA exists in moving liquids and needs to resist twisting due to the development of turbulent wakes of the fluids passing around it. Marko (1997) showed a strong coupling between stretching and twisting of the double helix. It is clear that the assessment of the response of DNA under tension is important. When DNA is in ambient tension of more than about $F_0 \cong 10$ pN, its material behavior changes from entropy-dominated to elasticity (enthalpy)-dominated (Smith et al., 1992). Theoretically, this limit tensile force has been calculated to be (Odijk, 1995)

$$F_0 = K_B T_a \left(\frac{\pi E}{16 K_B T_a} \right)^{1/3}, \quad (3)$$

where K_B is the Boltzmann constant, T_a is the absolute temperature, and E is the linear elastic Young's modulus. Regarding the elastic modulus E, Baumann et al. (1997) found that it depends on the ionic strength of the monovalent salt in the surrounding the DNA fluid. They report that when the applied tensile force $F$is larger than a value $F_0 \cong 10$pN at ambient temperature, the stretch modulus for λ-DNA in a solution containing 93 mM Na^+ is $S = 1006$pN. They also report the Poisson's ratio to be in the range $0 < \nu < 0.4$. Linear theory applies as soon as the molecule untangles under a very low load, as predicted by Eq. (3). Prior to that the molecule is coiled and the deformation follows the statistical mechanics random walk models (entropic mechanics), which also accounts for large deformations due to untanglement. We are not, however interested in that part of the deformation. Our concern is at higher loads when the DNA response is "linear" and "elastic", as suggested by the tests (enthalpic elasticity).

The topology of the DNA molecule is shown in Fig. 1; it shows a cross section that resembles a thin-walled open cross section rather than a circular cross section that almost all investigators have assumed so far. The structural form of the DNA molecule resembles that of a beam, with its cross section geometry often assumed to be circular with radius of 1 nm (Bao, 2002). However, a closer look at the shape of DNA (see for example Cluzel et al., 1996) shows that, after some stretching of the grooves of the helical coiling, its cross section appears approximately as an orthogonal.

The non-circular cross section of a beam produces out-of-plane deformation of the cross section (warping). If warping is constrained at one end, the elastic response changes drastically due to torsional coupling, even though no macroscopic torsional moment is applied at the ends of the beam. The analysis depends critically on the end boundary conditions. We formulate the problem of tension of pretwisted DNA by using the proposed structural gradient elasticity theory. Then, we solve the problem of tensile force-induced-torsion and give approximate closed form estimates for the overall deformation and strength of the DNA beam model.

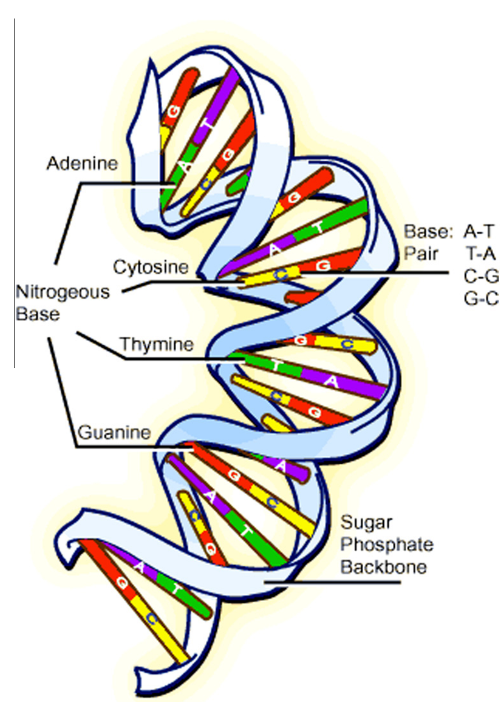

Fig. 1. Topology of the DNA molecule. Two strands of sugar-phosphate backbone form a double helix. The strands hold together with nitrogenous bases that form specific pairs through hydrogen bonds. (www.scq.ubc.ca/wp-content/dna.gif).

2. Multipolar elasticity analogue for the torsion problem of thin-walled beams – Uniform versus non-uniform torsion

We consider a cylindrical beam an open thin-walled cross section, which is constant along the beam. We introduce a Cartesian coordinate system *Oxyz* with the *z*-direction along the axis of the cylindrical beam and parallel to its generators. The beam is assumed to be of length L and one of its bases is taken to lie on the *xy*-plane, where $z = 0$. The beam is loaded in torsion by couples, the moments of which are normal to the bases of the cylinder. The torque T may or may not be uniform along the beam. The lateral surface of the cylinder is traction free. The material of the beam is homogeneous, isotropic, linearly elastic, with Young's modulus E, Poisson ratio ν, and shear modulus $G = \frac{E}{2(1+\nu)}$.

On each cross section, the arc length s is measured along the middle line C in the counterclockwise direction, starting from one end of the section, where $s = 0$. At each point on the middle line C, we introduce a normal direction normal n, in such a way that the system nsz is right-handed, with $n = 0$ on C and $-\frac{t(s)}{2} \leqslant n \leqslant \frac{t(s)}{2}$, where $t(s)$ is the thickness of the cross section normal to the middle line. The beam is thin-walled in the sense that the maximum value of $t(s)$ along C is small compared to the dimensions of the cross section (see for example Fig. 2).

2.1. Uniform torsion

We consider first the case in which the applied torque T is constant along the beam and all cross sections of the beam are free to warp. In that case, we have the classical Saint–Venant solution, in which the rotation ϕ about the z-axis of each cross section varies linearly along the beam, i.e., (e.g., Sokolnikoff, 1956)

$$\phi(z) = \phi_0 + \alpha z \text{ and } \frac{d\phi(z)}{dz} = \alpha = \text{const} \tag{4}$$

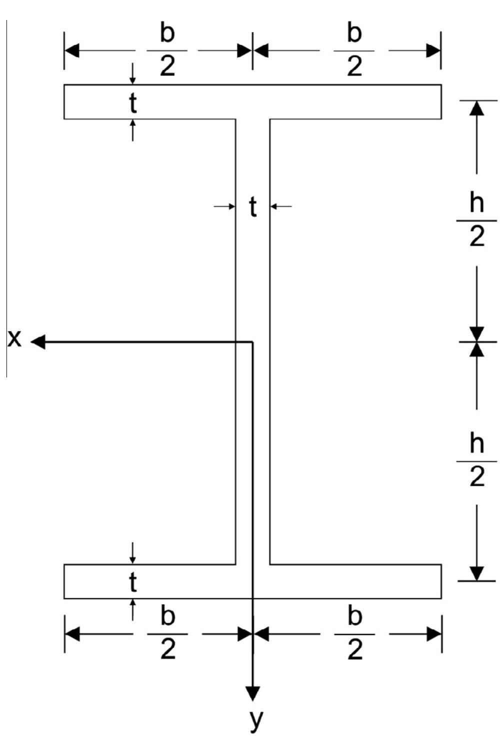

Fig. 2. Cross section of an I-beam.

where ϕ_0 is the rotation of the base at $z = 0$ of the beam and α is the constant twist per unit length of the beam. On each cross section at z, we define the average value of twist $\langle\phi\rangle_{z_0}$ as

$$\langle\phi\rangle_{z_0} = \frac{1}{\ell}\int_{z_0-\ell/2}^{z_0+\ell/2} \phi(z)dz, \tag{5}$$

where ℓ is a sampling length. Using Eq. (4) for $\phi(z)$, we can show readily that

$$\langle\phi\rangle_{z_0} = \phi(z_0), \tag{6}$$

i.e., the average value of twist $\langle\phi\rangle_{z_0}$ equals the local value $\phi(z_0)$.

The torque T is related to α by the well-known relationship

$$T = GJ\frac{d\phi}{dz} = GJ\alpha, \tag{7}$$

where $J = \frac{1}{3}\int_C t^3(s)ds$ is the torsional constant that depends on the shape of the cross section. Eq. (7) can be thought of as an elastic constitutive equation at the structure level that relates T to α.

Each cross section rotates rigidly in its plane by an angle $\phi(z)$ and warps; the axial displacement w of the points *along the middle line C* of the cross section is independent of z and can be written in the form

$$w(s) = w_0 - \alpha\omega(s), \tag{8}$$

where w_0 is a constant and $\omega(s)$ is the "sectorial area" of the middle line (e.g., Oden and Ripperger, 1981,Cook and Young, 1985). Points off the middle line experience an additional warping displacement w^{sec}, known as "secondary warping", which can become important in beams of "moderate" thickness. A detailed discussion of w^{sec} and the corresponding secondary stresses is given by Wagner (1936), see also Goodier (1962, p. 36–19) and Librescu and Song (2006, p. 18).

The axial strain $\varepsilon_{zz} = \frac{\partial w}{\partial z}$ vanishes along the middle line C. The only non-zero stress component is the shear stress σ_{sz}, which is practically independent of s (except near the "ends" of C) and varies linearly with n:

$$\sigma_{sz}(n) = \frac{2T}{J}n = 2Gn\frac{d\phi}{dz} = 2Gn\alpha. \tag{9}$$

The shear flow vanishes in this case, i.e.,

$$\int_{-t(s)/2}^{t(s)/2} \sigma_{sz}(n)dn = 0. \tag{10}$$

The elastic strain energy per unit length of the beam $\bar{U}$ is

$$\bar{U} = \frac{1}{2}T\frac{d\phi}{dz} = \frac{1}{2}T\alpha. \tag{11}$$

Fig. 2 shows the cross section of an I-beam with a flange width b, web height h, and thickness t. A schematic representation of the distribution of σ_{sz} on the cross section of an I-beam and the corresponding torque are shown in Fig. 3.

2.2. Non-uniform torsion – restrained warping – Vlasov's theory

We consider next the case in which the applied torque varies along the beam and/or the end cross sections are constrained so that they cannot warp freely. This problem has been addressed in detail by Vlasov in the 1940s in his pioneering work on thin-walled beams with open cross sections (Vlasov, 1969). That work is based on two main assumptions:

(i) the cross sections are rigid in their own planes, but they can warp out of their original planes and,
(ii) the shear strain ε_{sz} vanishes along the middle line.

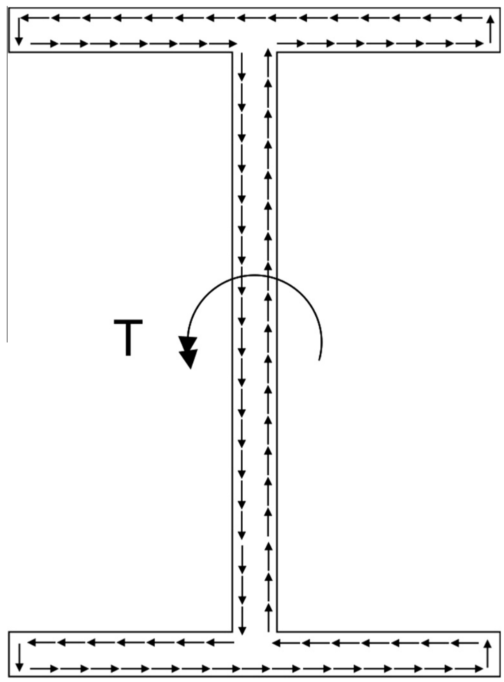

Fig. 3. Shear stress distribution according to the Saint–Venant theory of torsion.

There are two main differences between the non-uniform case and the uniform case described in Section 2.1:

(i) the twist $\phi(z)$ is a non-linear function of z and,
(ii) the axial displacement w depends on z; in fact, *along the middle line* of the cross section, w can be written in the form (Vlasov 1969)

$$w(s,z) = w_0 - \frac{d\phi(z)}{dz}\omega^*(s) \quad \text{on } C, \tag{12}$$

where w_0 is a constant and $\omega^*(s)$ is the "principal sectorial area" of the middle line, which is determined with a sectorial pole that is coincident with the "shear center" of the open thin-walled cross section (principal pole) and a sectorial origin on the middle line such that the integral of $\omega^*(s)$ along the middle line vanishes (principal origin), i.e., $\int_A \omega^* dA = 0$ (Cook and Young, 1985).

Since the axial displacement w depends onz, there exist axial strains ε_{zz}, which take the values

$$\varepsilon_{zz}(s,z) = \frac{\partial w(s,z)}{\partial z} = -\frac{d^2\phi(z)}{dz^2}\omega^*(s) \quad \text{on } C. \tag{13}$$

The corresponding axial stress σ_{zz} is

$$\sigma_{zz}(s,z) = E\varepsilon_{zz}(s,z) = -E\frac{d^2\phi(z)}{dz^2}\omega^*(s) \quad \text{on } C. \tag{14}$$

In view of the small thickness $t(s)$, the axial strain ε_{zz} and the corresponding bending stress σ_{zz} are assumed to be constant through the thickness of the cross section. Note that the following area integrals vanish:

$$\int_A \sigma_{zz} dA = 0, \quad \int_A x\sigma_{zz} dA = \int_A y\sigma_{zz} dA = 0, \tag{15}$$

$$\int_A \frac{\partial \sigma_{zz}}{\partial z} dA = 0, \quad \int_A x\frac{\partial \sigma_{zz}}{\partial z} dA = \int_A y\frac{\partial \sigma_{zz}}{\partial z} dA = 0, \tag{16}$$

where A is the area of the cross section. According to the above equations, the stress field σ_{zz} and the partial derivative $\frac{\partial \sigma_{zz}}{\partial z}$ are self-equilibrated, in the sense that the corresponding axial force N and bending moments M_x and M_y on the cross section vanish.

Since the quantity $\frac{\partial \sigma_{zz}}{\partial z}$ does vanish, there is a non-zero shear flow $q^\omega(s,z)$ on the cross section, and the total shear stress σ_{sz} is

$$\sigma_{sz}(n,s,z) = \sigma_{sz}^{SV}(n,z) + \sigma_{sz}^{\omega}(s,z) = \frac{2T^{SV}(z)}{J}n + \frac{q^\omega(s,z)}{t(s)}, \tag{17}$$

where the superscript SV indicates that the corresponding quantity is calculated by using the Saint–Venant theory and the superscript ω denotes quantities that appear due to the non-uniformity of $\frac{d\phi(z)}{dz}$. We also have that (e.g., see Vlasov, 1969; Oden and Ripperger, 1981; Cook and Young, 1985; Chen and Atsuta, 2007)

$$T = T^{SV}(z) + T^{\omega}(z), \quad T^{SV}(z) = GJ\frac{d\phi(z)}{dz}, \quad T^{\omega}(z) = -EJ_\omega\frac{d^3\phi(z)}{dz^3}, \tag{18}$$

where

$$J_\omega = \int_A \omega^{*2} dA \tag{19}$$

is the sectorial moment of the cross section with dimensions length raised to the sixth power.

Eq. (18) are a generalization of Eq. (7) and, again, can be thought of as elastic constitutive equations at the structure level.

The elastic strain energy per unit length of the beam $\bar{U}$ is

$$\bar{U}(z) = \int_A \left[\frac{(\sigma_{sz}^{SV})^2}{2G} + \frac{\sigma_{zz}^2}{2E}\right] dA = \frac{GJ}{2}\left[\frac{d\phi(z)}{dz}\right]^2 + \frac{EJ_\omega}{2}\left[\frac{d^2\phi(z)}{dz^2}\right]^2. \tag{20}$$

The "bimoment" (or "warping moment") B is also defined as (Vlasov, 1969)

$$B(z) = \int_A \sigma_{zz}(s,z)\omega^*(s) dA(s) = -EJ_\omega\frac{d^2\phi(z)}{dz^2} \tag{21}$$

and has dimensions of moment×length raised to the power two. A bimoment consists of equal and opposite moments acting about the same axis and separated from one another; its value is the product of the moment and the separation distance. The effect of a bimoment is to warp cross sections and twist the beam. The notion of the bimoment will become clear in the example of the I-beam that follows.

In view of Eq. (21) that defines the bimoment B, the torque Eq. (18) and the expression (20) for the elastic strain energy per unit length of the beam $\bar{U}(z)$ can be written in the form

$$T(z) = GJ\frac{d\phi(z)}{dz} + \frac{dB(z)}{dz} \tag{22}$$

and

$$\bar{U}(z) = \frac{1}{2}T^{SV}(z)\frac{d\phi(z)}{dz} - \frac{1}{2}B(z)\frac{d^2\phi(z)}{dz^2}. \tag{23}$$

Note that the pairs $\left(T, \frac{d\phi}{dz}\right)$ and $\left(B, -\frac{d^2\phi}{dz^2}\right)$ are "work conjugate".

For the special case of an I-beam with a flange widthb, web height h, and thickness t (Fig. 2), we have that

$$\omega^*(x,y) = \begin{cases} \frac{h}{2}x & \text{for } y = -\frac{h}{2}, \\ 0 & \text{for } -\frac{h}{2} < y < \frac{h}{2}, \\ -\frac{h}{2}x & \text{for } y = \frac{h}{2}, \end{cases}$$
$$\sigma_{zz}(x,y,z) = E\frac{d^2\phi(z)}{dz^2}\begin{cases} -\frac{h}{2}x & \text{for } y = -\frac{h}{2}, \\ 0 & \text{for } -\frac{h}{2} < y < \frac{h}{2}, \\ \frac{h}{2}x & \text{for } y = \frac{h}{2}, \end{cases} \tag{24}$$

where the x-y axes are as shown in Fig. 2.

A schematic representation of the stresses that develop on the cross section is shown in Fig. 4.

The sectorial moment of the cross section and the bimoment for the I-beam are

$$J_\omega = \int_A \omega^{*2} dA = \frac{1}{24} b^3 h^2 t, \text{ and } B = \int_A \sigma_{zz} \omega^* dA = -\frac{Eb^3 h^2 t}{24} \frac{d^2\phi}{dz^2}. \quad (25)$$

Fig. 5 shows the corresponding cross section resultant moments T^{SV}, T^{ω} and M_f for the I-beam. The bending moments shown on the flanges of the cross section are

$$\mathbf{M}_{upper} = -\mathbf{M}_{lower} = M_f \mathbf{e}_y, \quad M_f = -\int_{-b/2}^{b/2} x\sigma_{zz}|_{y=-\frac{h}{2}} dx = \frac{Eb^3 ht}{24} \frac{d^2\phi}{dz^2}, \quad (26)$$

where e_y is the unit vector along the $y-$axis. The bending moments M_f correspond to the axial stresses $\sigma_z z$ shown in Fig. 5 that develop on the flanges due to the non-uniformity of $\frac{d\phi}{dz}$. The equal and opposite bending moments M_f cause additional warping of the cross section and create the bimoment B:

$$B = -M_f h = -\frac{Eb^3 h^2 t}{24} \frac{d^2\phi}{dz^2}. \quad (27)$$

2.3. A gradient elasticity formulation for restrained torsion and its connection to Vlasov's theory – The case of an I-beam

Here, we follow Vardoulakis and Giannakopoulos (2006), who considered the bending problem of a T-beam, and present an alternative formulation for the problem of restrained torsion in the context of a structural strain gradient elasticity theory. At the end of this section, we consider the example of an I-beam.

The twist of the cross sections in the neighbor of $z = z_0$ is approximated by a two-term Taylor series expansion:

$$\phi(z) \cong \phi(z_0) + \left(\frac{d\phi}{dz}\right)_{z=z_0} (z - z_0) + \frac{1}{2}\left(\frac{d^2\phi}{dz^2}\right)_{z=z_0} (z - z_0)^2. \quad (28)$$

The average twist of the cross sections in the region $z_0 - \frac{\bar{\ell}}{2} \leqslant z \leqslant z_0 + \frac{\bar{\ell}}{2}$ is

$$\langle\phi\rangle_0 = \frac{1}{\bar{\ell}} \int_{z_0-\bar{\ell}/2}^{z_0+\bar{\ell}/2} \phi(z) dz \cong \phi(z_0) + \frac{\bar{\ell}^2}{24}\left(\frac{d^2\phi}{dz^2}\right)_{z=z_0} \text{ so that } \phi(z_0) \cong \langle\phi\rangle_0 - \frac{\bar{\ell}^2}{24}\left(\frac{d^2\phi}{dz^2}\right)_{z=z_0}, \quad (29)$$

where $\bar{\ell}$ is a "structural length" to be defined later. The above equation shows that the local value $\phi(z_0)$ can differ substantially from the corresponding local average value $\langle\phi\rangle_0$, when the term $\frac{\bar{\ell}^2}{24}\left(\frac{d^2\phi}{dz^2}\right)_{z=z_0}$ is not negligible compared to $\langle\phi\rangle_0$. In classical "simple theories", local field variables are identified with mean values and the corresponding continua are described as locally homogeneous. However, when the local variation of variables is significant (so that terms such as $\frac{\bar{\ell}^2}{24}\left(\frac{d^2\phi}{dz^2}\right)_{z=z_0}$ are comparable to $\langle\phi\rangle_0$), higher order theories are more appropriate. In that context, we propose to replace the twist ϕ in the structural constitutive Eq. (7) by $\phi - \ell^2 \frac{d^2\phi}{dz^2}$ with $\ell = \frac{\bar{\ell}}{\sqrt{24}}$, so that

$$T(z) = GJ \frac{d}{dz}\left[\phi(z) - \ell^2 \frac{d^2\phi(z)}{dz^2}\right] = GJ\left[\frac{d\phi(z)}{dz} - \ell^2 \frac{d^3\phi(z)}{dz^3}\right]. \quad (30)$$

The above relationship can be viewed as an elastic structural constitutive equation of the "strain gradient type". Eq. (30) is identical to Eq. (18) of Vlasov's theory, provided that we identify $\ell^2 GJ$ with the "warping rigidity" EJ_ω, i.e.,

$$\ell = \sqrt{\frac{E}{G}\frac{J_\omega}{J}} = \sqrt{2(1+\nu)\frac{J_\omega}{J}} \text{ or } J_\omega = \ell^2 \frac{G}{E} J = \ell^2 \frac{J}{2(1+\nu)}. \quad (31)$$

The results of the previous section can be recast now in the context of a linearly elastic strain gradient formulation. The strain energy per unit length of the beam that corresponds to the axial stress σ_{zz} is (see Eq. (20))

$$\bar{U}_{\sigma_{zz}} \equiv \int_A \frac{\sigma_{zz}^2}{2E} dA = \frac{EJ_\omega}{2}\left(\frac{d^2\phi}{dz^2}\right)^2 = -\frac{1}{2} B \frac{d^2\phi}{dz^2} \equiv \frac{1}{2} B\bar{\bar{\kappa}}, \quad (32)$$

where

$$\bar{\bar{\kappa}} \equiv -\frac{d^2\phi}{dz^2}. \quad (33)$$

Then, the structural "gradient elasticity" equations for the restrained torsion problem of the I-beam can be written as follows

$$\text{equilibrium}: T = T^{SV} + \frac{dB}{dz}, \quad \frac{dT}{dz} = -m_z, \quad (34)$$

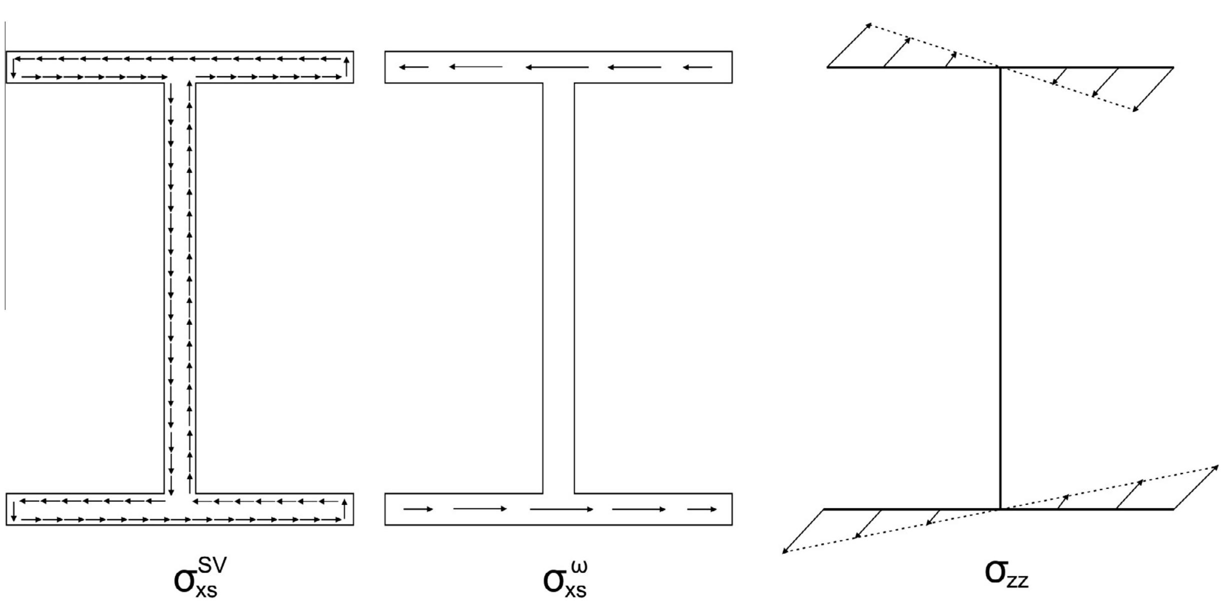

Fig. 4. Shear and normal stresses on an I-beam. The direction of σ_{zz} corresponds to the case where $d^2\phi/dz^2 > 0$.

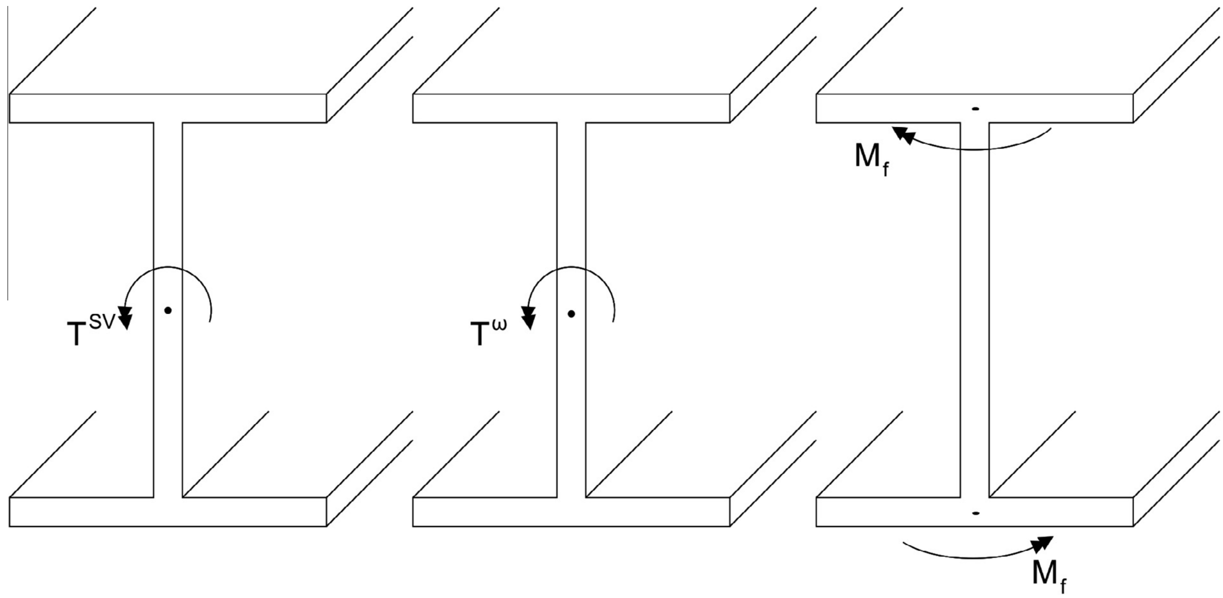

Fig. 5. Resultant moments on the cross section of an I-beam. Note that T^{SV} and T^{ω} correspond to couples acting on the plane of the cross section (torsion about the z-axis), whereas M_f corresponds to a couple acting on the plane of the web (bending about the y-axis).

$$\text{compatibility}: \ \alpha = \frac{d\phi(z)}{dz}, \quad \bar{\bar{\kappa}} = -\frac{d\alpha(z)}{dz}, \tag{35}$$

$$\text{constitutive}: T^{SV}(\alpha) = GJ\alpha, \quad B(\bar{\bar{\kappa}}) = \ell^2 GJ\bar{\bar{\kappa}}, \tag{36}$$

$$\text{elastic strain energy density}: \bar{U}(\alpha, \bar{\bar{\kappa}}) = \frac{GJ}{2}(\alpha^2 + \ell^2\bar{\bar{\kappa}}^2), \tag{37}$$

so that

$$T^{SV} = \frac{\partial \bar{U}}{\partial \alpha}, \quad B = \frac{\partial \bar{U}}{\partial \bar{\bar{\kappa}}} \text{ and } \bar{U} = \frac{1}{2}T^{SV}\alpha + \frac{1}{2}B\bar{\bar{\kappa}}. \tag{38}$$

In Eq. (34b), m_z is the distributed torsion per unit length of the beam.

Combining the above equations, we conclude that the governing differential equation for $\phi(z)$ is

$$\frac{d^2\phi}{dz^2} - \ell^2\frac{d^4\phi}{dz^4} = -\frac{m_z}{GJ}. \tag{39}$$

In order to derive the appropriate boundary conditions for the above differential equation, we present in the following section a variational formulation of the problem.

For the special case of an I-beam with a flange width b, web height h, and thickness t (Fig. 2), we have that

$$J = \frac{1}{3}(2b+h)t^3, \ J_\omega = \frac{1}{24}b^3h^2t, \ \ell = \sqrt{\frac{EJ_\omega}{GJ}} = \sqrt{\frac{E/G}{2(2+\frac{h}{b})}}\frac{bh}{2t}, \tag{40}$$

$$\varepsilon_{zz}(x,y,z) = \frac{d^2\phi(z)}{dz^2}\begin{cases} -\frac{h}{2}x & \text{for } y = -\frac{h}{2}, \\ 0 & \text{for } -\frac{h}{2} < y < \frac{h}{2}, \\ \frac{h}{2}x & \text{for } y = \frac{h}{2}. \end{cases} \tag{41}$$

$$\kappa_{zzx}(y,z) \equiv \frac{\partial \varepsilon_{zz}}{\partial x} = \begin{cases} -\frac{h}{2}\frac{d^2\phi(z)}{dz^2} & \text{for } y = -\frac{h}{2}, \\ 0 & \text{for } -\frac{h}{2} < y < \frac{h}{2}, \\ \frac{h}{2}\frac{d^2\phi(z)}{dz^2} & \text{for } y = \frac{h}{2} \end{cases} \tag{42}$$

and

$$\bar{\bar{\kappa}} = -\frac{d^2\phi}{dz^2} = -\frac{1}{h}\left(\kappa_{zzx}|_{y=\frac{h}{2}} - \kappa_{zzx}|_{y=-\frac{h}{2}}\right). \tag{43}$$

Following Vardoulakis and Giannakopoulos (2006), who considered "double forces", we give a geometric picture of the "double moments" introduced by Mindlin (1964). Referring to Fig. 4, where the cross section moments are shown for an I-beam, we note that the self-equilibrated bending moments M_f on the flanges are essentially "double moments" which are responsible for the bimoment $B = -M_f h$ and contribute to the elastic strain energy of the beam U (see eqn (38b)).

3. Variational formulation, boundary conditions and general solution – The pretwist

Having the DNA problem in mind, we include the effects of "pretwist" in the variational formulation of the problem. In particular, we consider the problem of torsion in an initially twisted thin-walled beam of the type described in Section 2. The initial twist is described by a rotation $\phi_0(z)$ of each cross section about the $z-$axis. The function $\phi_0(z)$ is linear in z:

$$\phi_0(z) = \alpha_0 z, \tag{44}$$

where α_0 is the constant rate of pretwist. The initial pretwisted state is stress free.

A thorough review of the structural and dynamic behavior of pretwisted rods and beams has been given by Rosen (1991). Following Rosen (1978, 1980), we introduce on each cross section at z, a local coordinate system $\eta - \zeta$ by rotating the global x-y axes about the z-axis by an angle $\phi_0(z)$. Then the analytical expression that describes the boundary of each cross section relative to the $\eta - \zeta$ system is the same for z. On each cross section at z, we have the embedded coordinates

$$\begin{aligned} \eta(x,y,z) &= x\cos\phi_0(z) + y\sin\phi_0(z), \\ \zeta(x,y,z) &= -x\sin\phi_0(z) + y\cos\phi_0(z), \end{aligned} \tag{45}$$

so that

$$\frac{\partial \eta}{\partial z} = \alpha_0\zeta \text{ and } \frac{\partial \zeta}{\partial z} = -\alpha_0\eta. \tag{46}$$

The axial displacement w is written in the form Rosen (1978) and Rosen (1980)

$$w(x,y,z) = w_1(z) + \frac{d\phi(z)}{dz}\Psi(\eta(x,y,z),\zeta(x,y,z)), \tag{47}$$

where $\Psi(\eta,\zeta)$ is the usual Saint–Venant warping function, $w_1(z)$ and $\phi(z)$ are the basic kinematic unknowns, s is the arc length measured along the middle line as before. The classical problem with no pretwist is recovered if we set $w_1(z) = w_0 =$constant and $\phi_0(z) = 0$, so that $\eta = x$ and $\zeta = y$.

In thin-walled cross sections, the warping function Ψ can be identified (to first order) with the negative of the principal sectorial area ω^*, i.e., $\Psi = -\omega^*$; when the thickness is moderate, additional terms that account for the through the thickness variation of Ψ can be included (secondary warping) as discussed in Section 4.

On a thin-walled cross section, the only non-zero strain components are

$$\varepsilon_{zs}(n,z) = n\frac{d\phi(z)}{dz} \text{ and } \varepsilon_{zz}(n,s,z) = \frac{\partial w}{\partial z} = \frac{d^2\phi}{dz^2}\Psi + \frac{dw_1}{dz} + \frac{d\phi}{dz}\frac{\partial\Psi}{\partial z}, \tag{48}$$

where n is again the coordinate normal to the middle line and

$$\frac{\partial\Psi}{\partial z} = \frac{\partial\Psi}{\partial\eta}\frac{\partial\eta}{\partial z} + \frac{\partial\Psi}{\partial\zeta}\frac{\partial\zeta}{\partial z} = \alpha_0\left(\zeta\frac{\partial\Psi}{\partial\eta} - \eta\frac{\partial\Psi}{\partial\zeta}\right). \tag{49}$$

The last two terms in the expression (48b) for the axial strain are due to pretwist (compare to Eq. (13)).

The elastic stain energy per unit length of the beam is

$$\bar{U}(z) = \int_A \left(\frac{E}{2}\varepsilon_{zz}^2 + 2G\varepsilon_{zs}^2\right)dA = \bar{U}_0 + \bar{U}^{\text{pretwist}}, \tag{50}$$

where

$$\bar{U}_0(\phi(z)) = \frac{GJ}{2}\left[\left(\frac{d\phi}{dz}\right)^2 + \ell^2\left(\frac{d^2\phi}{dz^2}\right)^2\right], \tag{51}$$

$$\bar{U}^{\text{pretwist}}(\phi(z),w_1(z)) = \frac{EA}{2}\left[\left(\frac{dw_1}{dz}\right)^2 + \frac{\alpha_0^2K}{A}\left(\frac{d\phi}{dz}\right)^2 + 2\frac{\alpha_0 S}{A}\frac{dw_1}{dz}\frac{d\phi}{dz} + 2\frac{\alpha_0 R}{A}\frac{d\phi}{dz}\frac{d^2\phi}{dz^2}\right], \tag{52}$$

with

$$\alpha_0^2K = \int_A\left(\frac{\partial\Psi}{\partial z}\right)^2 dA, \quad \alpha_0 R = \int_A \Psi\frac{\partial\Psi}{\partial z}dA, \quad \alpha_0 S = \int_A \frac{\partial\Psi}{\partial z}dA. \tag{53}$$

Non-zero values of K, R, and S are due to pretwist and are associated with the $z-$dependence of the warping function Ψ.

Remarks:

(1) If we use Schwartz's inequality (e.g., Hardy et al., 1952, p. 133)

$$\left(\int_A fg dA\right)^2 \leqslant \left(\int_A f^2 dA\right)\left(\int_A g^2 dA\right) \tag{54}$$

with $f = \frac{\partial\Psi}{\partial z}$ and $g = 1$, we conclude that

$$\left(\int_A \frac{\partial\Psi}{\partial z}dA\right)^2 \leqslant A\int_A\left(\frac{\partial\Psi}{\partial z}\right)^2 dA. \tag{55}$$

The last equality implies that

$$S^2 \leqslant AK. \tag{56}$$

(2) If we take into account that the warping function Ψ is harmonic $\left(\nabla^2\Psi = 0\right)$ and satisfies the condition $\frac{\partial\Psi}{\partial n} = \zeta n_\eta - \eta n_\zeta$ on the boundary ∂A of the cross section, where $\mathbf{n}$ is the outward unit normal and $\frac{\partial\Psi}{\partial n} = \nabla\Psi\cdot\mathbf{n}$, we can show that $S \geqslant 0$. The proof is as follows (see also Corradi Dell'Acqua, 1992, p. 301):

$$\begin{aligned}
S &= \frac{1}{\alpha_0}\int_A \frac{\partial\Psi}{\partial z}dA = \int_A\left(\zeta\frac{\partial\Psi}{\partial\eta} - \eta\frac{\partial\Psi}{\partial\zeta}\right)dA \\
&= \int_A\left[\frac{\partial}{\partial\eta}(\zeta\Psi) - \frac{\partial}{\partial\zeta}(\eta\Psi)\right]dA = \oint_{\partial A}\Psi(\zeta n_\eta - \eta n_\zeta)ds \\
&= \oint_{\partial A}\Psi\frac{\partial\Psi}{\partial n}ds = \oint_{\partial A}\left(\Psi\frac{\partial\Psi}{\partial\eta}n_\eta + \Psi\frac{\partial\Psi}{\partial\zeta}n_\zeta\right)ds \\
&= \int_A\left[\frac{\partial}{\partial\eta}\left(\Psi\frac{\partial\Psi}{\partial\eta}\right) + \frac{\partial}{\partial\zeta}\left(\Psi\frac{\partial\Psi}{\partial\zeta}\right)\right]dA \\
&= \int_A\left[\left(\frac{\partial\Psi}{\partial\eta}\right)^2 + \left(\frac{\partial\Psi}{\partial\zeta}\right)^2 + \nabla^2\Psi\right]dA \\
&= \int_A\left[\left(\frac{\partial\Psi}{\partial\eta}\right)^2 + \left(\frac{\partial\Psi}{\partial\zeta}\right)^2\right]dA \geqslant 0,
\end{aligned}$$

where the boundary condition $\frac{\partial\Psi}{\partial n} = \zeta n_\eta - \eta n_\zeta$ and the divergence theorem have been used. □

The total elastic strain energy U of the beam is

$$U = \int_0^L \bar{U}(z)dz. \tag{57}$$

We will obtain the governing equations and the corresponding boundary conditions by minimizing the total potential $U - W$:

$$\delta(U - W) = 0, \tag{58}$$

where the external work W includes the total torque T, the axial load N, the bimoment B, the distributed axial loads per unit length $p_z = -\frac{dN}{dz}$, and the distributed torsional moments per unit length $m_z = -\frac{dT}{dz}$, so that

$$\delta W = \int_0^L (p_z\delta w_1 + m_z\delta\phi)dz + (N\delta w_1)_0^L + (T\delta\phi)_0^L + \left(-B\frac{d\delta\phi}{dz}\right)_0^L. \tag{59}$$

Taking the variation of U from (57) and using (59), we obtain:

$$\begin{aligned}
\delta(U-W) = &\int_0^L\left\{\left[-E\ \ A\frac{d^2w_1}{dz^2} + \alpha_0 S\frac{d^2\phi}{dz^2}\Bigg) - p_z\right]\delta w_1\right\}dz \\
&+ \int_0^L\left\{\left[GJ\ \ \ell^2\frac{d^4\phi}{dz^4} - \frac{d^2\phi}{dz^2}\Bigg) - E\ \ \alpha_0^2K\frac{d^2\phi}{dz^2} + \alpha_0 S\frac{d^2w_1}{dz^2}\Bigg) - m_z\right]\delta\phi\right\}dz \\
&+ \left\{\left[E\left(A\frac{dw_1}{dz} + \alpha_0 S\frac{d\phi}{dz}\right) - N\right]\delta w_1\right\}_0^L \\
&+ \left\{\left[GJ\ \ -\ell^2\frac{d^3\phi}{dz^3} + \frac{d\phi}{dz}\Bigg) + E\left(\alpha_0^2K\frac{d\phi}{dz} + \alpha_0 S\frac{dw_1}{dz}\right) - T\right]\delta\phi\right\}_0^L \\
&+ \left[\ \ \ell^2 GJ\frac{d^2\phi}{dz^2} + \alpha_0 ER\frac{d\phi}{dz} + B\Bigg)\frac{d\delta\phi}{dz}\right]_0^L.
\end{aligned} \tag{60}$$

In view of (58), we conclude that the governing equations for $\phi(z)$ and $w_1(z)$ are

$$\frac{d^2w_1}{dz^2} + \frac{\alpha_0 S}{A}\frac{d^2\phi}{dz^2} = -\frac{p_z}{EA}, \tag{61}$$

$$\ell^2\frac{d^4\phi}{dz^4} - \left(1 + \frac{E}{G}\frac{\alpha_0^2K}{J}\right)\frac{d^2\phi}{dz^2} - \frac{E}{G}\frac{\alpha_0 S}{J}\frac{d^2w_1}{dz^2} = \frac{m_z}{GJ}. \tag{62}$$

The boundary conditions resulting from (58) are that at the two ends of the beam we can describe

(i) either the twist $\phi = \bar{\phi} =$ known or

$$\text{the torque } \left(1+\alpha_0^2 \frac{E}{G}\frac{K}{J}\right)\frac{d\phi}{dz} - \ell^2 \frac{d^3\phi}{dz^3} + \alpha_0 \frac{E}{G}\frac{S}{J}\frac{dw_1}{dz} = \frac{\bar{T}}{GJ} = \text{known}, \tag{63}$$

(ii) either the rate of twist $\frac{d\phi}{dz} = \bar{\phi}\prime =$ known or

$$\text{the bimoment } \ell^2 \frac{d^2\phi}{dz^2} + \alpha_0 \frac{E}{G}\frac{R}{J}\frac{d\phi}{dz} = -\frac{\bar{B}}{GJ} = \text{known}, \tag{64}$$

(iii)

either the axial displacement $w_1 = \bar{w}_1 =$ known or

$$\text{the axial force } \frac{dw_1}{dz} + \alpha_0 \frac{S}{A}\frac{d\phi}{dz} = \frac{\bar{N}}{EA} = \text{known}. \tag{65}$$

Remark: The pretwist α_0 modifies the equations for the axial force, the torque, and the bimoment. In fact, (61) and (62) imply that

$$N(z) = E\left[A\frac{dw_1(z)}{dz} + \alpha_0 S \frac{d\phi(z)}{dz}\right] \text{ and } T(z) = T^{SV}(z) + T^{\omega}(z) + T^{\text{pretwist}}(z), \tag{66}$$

where

$$T^{SV}(z) = GJ\frac{d\phi(z)}{dz}, \quad T^{\omega}(z) = -\ell^2 GJ \frac{d^3\phi(z)}{dz^3}, \quad T^{\text{pretwist}}(z) = \alpha_0 E\left[\alpha_0 K \frac{d\phi(z)}{dz} + S\frac{dw_1(z)}{dz}\right]. \tag{67}$$

The bimoment is now defined by Eq. (64):

$$B(z) = -\left[\ell^2 GJ \frac{d^2\phi(z)}{dz^2} + \alpha_0 RE \frac{d\phi(z)}{dz}\right]. \tag{68}$$

The terms that involve α_0 in (66)–(68) are due to pretwist. □

We can combine (61) and (62) to eliminate $w_1(z)$. The resulting differential equation for $\phi(z)$ is

$$\left(\frac{\ell^2}{c^2}\frac{d^2}{dz^2} - 1\right)\frac{d^2\phi(z)}{dz^2} = \frac{f(z)}{GJ_{\text{eff}}}, \quad \text{where } f(z) = m_z(z) - \alpha_0 \frac{S}{A} p_z(z) \tag{69}$$

and

$$c^2 = 1 + \alpha_0^2 \frac{E}{G}\frac{KA - S^2}{AJ} \equiv \frac{J_{\text{eff}}}{J}. \tag{70}$$

The constant c is dimensionless and accounts for the effects of pretwist; in the case of no pretwist $(\alpha_0 = 0), c = 1$ and $J_{\text{eff}} = J$.

Note that a Schrödinger-like operator appears in (69a); this is typical in strain-gradient beam problems (Vardoulakis and Giannakopoulos, 2006; Papargyri-Beskou et al., 2003). It should be noted also that the characteristic length ℓ multiplies the highest derivative in the differential Eq. (69). Therefore, the problem with a small $\ell \neq 0$ is a "singular perturbation" to the classical case $\ell = 0$. Boundary layers are known to develop at the ends of the beam for $\ell \neq 0$ and the limit of the solution as $\ell \to 0$ should be considered with care (Van Dyke, 1975).

The corresponding boundary conditions at the ends of the beam are

(i) either the twist $\phi = \bar{\phi} =$ known or

$$-\ell^2 \frac{d^3\phi}{dz^3} + c^2 \frac{d\phi}{dz} = \frac{\bar{T}}{GJ} - \alpha_0 \frac{S}{GJ}\frac{\bar{N}}{A} = \text{known}, \tag{71}$$

(ii) either the rate of twist $\frac{d\phi}{dz} = \bar{\phi}' =$ known or

$$\text{the bimoment } \ell^2 \frac{d^2\phi}{dz^2} + \alpha_0 \frac{E}{G}\frac{R}{J}\frac{d\phi}{dz} = -\frac{\bar{B}}{GJ} = \text{known}. \tag{72}$$

In deriving (71), we made the assumption that w_1 is not prescribed at either end of the beam.

The corresponding torque Eqs. (67c) and (66b) take the form

$$T^{\text{pretwist}}(z) = \alpha_0^2 E \frac{AK - S^2}{A}\frac{d\phi(z)}{dz} + \frac{\alpha_0 S}{A} N(z) \tag{73}$$

and

$$T(z) = GJ_{\text{eff}}\frac{d\phi(z)}{dz} - \ell^2 GJ \frac{d^3\phi(z)}{dz^3} + \frac{\alpha_0 S}{A} N(z). \tag{74}$$

Remark: In the classical theory $(\ell = 0)$ with no axial forces $(N = 0)$, the last equation becomes

$$T(z) = GJ_{\text{eff}}\frac{d\phi(z)}{dz}, \tag{75}$$

where $J_{\text{eff}} = \left(1 + \alpha_0^2 \frac{E}{G}\frac{AK - S^2}{A}\right)J \equiv c^2 J$ is the "effective torsional constant", as determined by Rosen (1980). In view of (56), we have that $J_{\text{eff}} > J$, i.e., pretwisting increases the torsional stiffness. □

The general solution of Eq. (69)a is

$$\phi(z) = A_1 + A_2 \frac{cz}{\ell} + A_3 \cosh\frac{cz}{\ell} + A_4 \sinh\frac{cz}{\ell} - \frac{\ell}{cGJ_{\text{eff}}}\int_0^z \left[\frac{c(z-\xi)}{\ell} - \sinh\frac{c(z-\xi)}{\ell}\right] f(\xi)d\xi. \tag{76}$$

The four dimensionless constants A_1, A_2, A_3 and A_4 are determined by the boundary conditions.

4. Tension of DNA

The structural form of the DNA molecule resembles that of a beam, with its shown schematically in Fig. 6. At the ends of the cross section $(x = +-b/2)$ are the "strands", which are the sugar phosphate backbone lines shown in Fig. 1. In-between are the nitrogenous bases, namely the A–T, T–A, C–G and G–C pairs between adenine (A), cytosine (C), thimine (T) and guanine (G). Referring to Fig. 6, we note that the corresponding dimensions are $b \cong 2$ nm and $t \cong 0.5$ nm, giving an approximate cross sectional area $A = bt \cong 1\text{ nm}^2$ (Bao, 2002). The reason for this slender shape is that the bases that connect the two strands are thin and, although they are from different matter than the strands, we have no data to distinguish them elastically. Therefore, a "homogenized" thin-walled cross section emerges in the modeling.

For this cross section, the ratio $\frac{t}{b} \cong 0.25$, i.e., the thickness of the cross section is "moderate". The torsional constant in this case can be approximated by

$$J \cong \frac{bt^3}{3}\left[1 - \frac{192}{\pi^5}\frac{t}{b} + \frac{16}{\pi^5}\left(\frac{t}{b}\right)^5\right]. \tag{77}$$

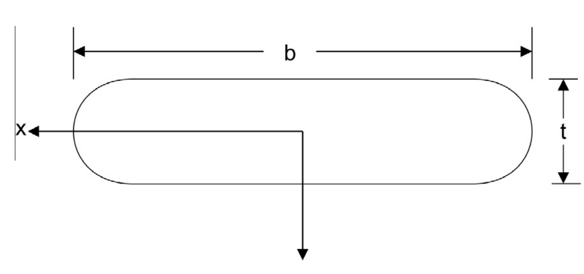

Fig. 6. Typical cross section of DNA. The strands are located at $x = \pm b/2$ and in-between are the base pairs (see also Fig. 1).

We note that, in thin-walled beams ($\frac{t}{b} \ll 1$), the sectorial area ω^* vanishes along the middle line of the cross section shown in Fig. 6; hence, the axial displacement w vanishes along the middle line, no warping torque T^{ω} can be developed and no longitudinal stresses are produced by torsional loads, if a thin-wall theory is used. However, when the thickness t is not extremely small compared to b, a secondary stress system can develop perpendicular to the middle line (see Oden and Ripperger, 1981, pp. 229–231). This secondary state of stress is associated with the axial displacement of points that are off the middle line on the cross section. Secondary axial stresses $\sigma_{zz}^{\sec}$ that vary linearly in the direction of the plane of bending on the cross section and shearing stress σ_{nz}^{ω} (normal to the middle line) can no longer be neglected, and a secondary warping torque $T_{\sec}^{\omega}$ develops. In such cases the cross section undergoes secondary warping and, consequently, possesses a secondary warping rigidity $EJ_{\omega}^{\sec}$. For sections such as this in Fig. 6, the only warping stresses developed due to twisting are the secondary stresses. A brief discussion of quantities associated to secondary warping is given in the Appendix.

Returning to the DNA problem, we note that the torsional moment of inertia in this case is secondary and is approximated by (e.g., Oden and Ripperger, 1981 and Rees, 2000)

$$J_{\omega} = J_{\omega}^{\sec} \cong \frac{b^3 t^3}{144}. \tag{78}$$

A rigorous derivation of (78) has been given by Rodríguez and Viaño (1993) and dell'Isola and Rosa (1994), who used asymptotic methods to determine a formal series expansion of the solution of the torsion problem in terms of a small parameter (the thickness t).

For the dimensions listed above, the corresponding values of J and J_{ω} are

$$J = 70.27 \times 10^{-3}\ \text{nm}^4 \text{ and } J_{\omega} = 6.944 \times 10^{-3}\ \text{nm}^6. \tag{79}$$

Based on the discussion of the Introduction, we conclude that a typical value for elastic modulus of DNA can calculated as

$$E = \frac{S}{A} = \frac{1006\ \text{pN}}{1\ \text{nm}^2} = 1006\ \text{MPa} \quad (\text{for } F > F_0), \tag{80}$$

a value that we will adopt in the present analysis. Assuming that the Poisson ratio takes the value $\nu = 0.25$, we find that the internal length in this case is

$$\ell = \sqrt{\frac{E}{G}\frac{J_{\omega}}{J}} = 0.497\ \text{nm}. \tag{81}$$

The constants (K, R, S), defined in Eq. (53), are associated with pretwisting and take the values (see Appendix)

$$K = \frac{b^5 t}{80}\left[1 - \frac{10}{9}\left(\frac{t}{b}\right)^2 + \left(\frac{t}{b}\right)^4\right] = 0.1869\ \text{nm}^6, \quad R = 0, \quad S = \frac{b^3 t}{12}\left[1 - \left(\frac{t}{b}\right)^2\right] = 0.3125\ \text{nm}^4. \tag{82}$$

Also, the constant c that defines the effective torsional stiffness in Eq. (75) is

$$c = \sqrt{\frac{J_{\text{eff}}}{J}} = \sqrt{1 + \alpha_0^2 \frac{E}{G}\frac{AK - S^2}{AJ}} = 1.0025. \tag{83}$$

We consider an almost straight DNA molecule of length L. A typical test of stretching of DNA by a magnetic device is shown schematically in Fig. 7. The two ends of the DNA are attached on a flat glass surface and on a magnetic bead respectively (Bao, 2002). In line with the actual experiments, we assume that at one end ($z = 0$) the molecule is fixed. At the other end $z = L$, a known rate of twist ϕ_L' is applied due to an axial tensile force F are applied. The $F - \phi_L'$ relation and the value of F required to unwind the DNA are discussed in this section.

In this problem $p_z(z) = 0$ and $m_z(z) = 0$; the axial force is constant and the torque vanishes, i.e., $N(z) = F$ and $T(z) = 0$. The corresponding boundary conditions for Eq. (69) are

$$\phi = 0 \text{ and } \frac{d\phi}{dz} = 0 \quad \text{at } z = 0, \tag{84}$$

and

$$-\ell^2 \frac{d^3\phi}{dz^3} + c^2 \frac{d\phi}{dz} = -\frac{\alpha_0 S}{J}\frac{F}{GA} \text{ and } \frac{d\phi}{dz} = \phi_L' \quad \text{at } z = L. \tag{85}$$

Such boundary conditions apply to actual experiments of combined stretching and torsion of DNA molecules, as shown in Fig. 7.

The general solution of the governing differential Eq. (69) is

$$\phi(z) = A_1 + A_2 \frac{cz}{\ell} + A_3 \cosh\frac{cz}{\ell} + A_4 \sinh\frac{cz}{\ell}. \tag{86}$$

The total torque vanishes, i.e., $T = T^{SV} + T^{\omega} + T^{\text{pretwist}} = 0$, and the individual components take the values

$$T^{SV} = \frac{cGJ}{\ell}\left(A_2 + A_3 \sinh\frac{cz}{\ell} + A_4 \cosh\frac{cz}{\ell}\right), \tag{87}$$

$$T^{\omega} = -\frac{c^3 GJ}{\ell}\left(A_3 \sinh\frac{cz}{\ell} + A_4 \cosh\frac{cz}{\ell}\right) \tag{88}$$

and

$$T^{\text{prerwist}} = -\alpha_0 S \frac{F}{A} + \frac{\alpha_0^2 cE}{\ell} \times \frac{AK - S^2}{A}\left(A_2 + A_3 \sinh\frac{cz}{\ell} + A_4 \cosh\frac{cz}{\ell}\right). \tag{89}$$

the corresponding bimoment is

$$B(z) = -c\left[A_2 \frac{\alpha_0^2 RE}{\ell} + \left(A_3 cGJ + A_4 \frac{\alpha_0^2 RE}{\ell}\right)\cosh\frac{cz}{\ell} + \left(A_3 \frac{\alpha_0^2 RE}{\ell} + A_4 cGJ\right)\sinh\frac{cz}{\ell}\right]. \tag{90}$$

The boundary conditions (84) and (85) define the constant (A_1, A_2, A_3, A_4):

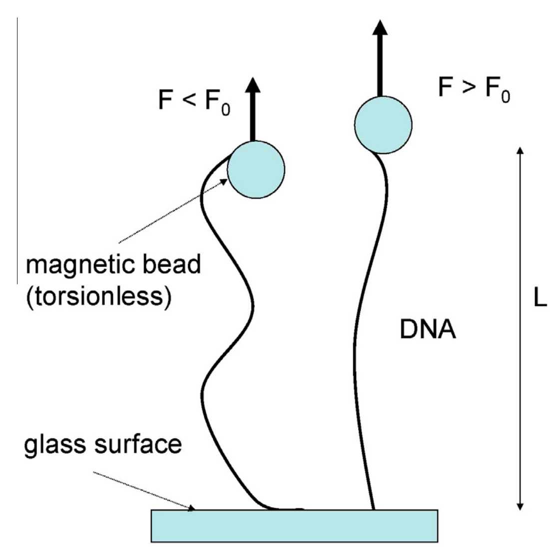

Fig. 7. Controlled stretch and twist using a magnetic device to pull DNA without exerting a torque.

$$A_2 = -A_4 = -\frac{\ell\alpha_0}{c^3}\frac{S}{J}\frac{F}{GA}, \quad A_1 = -A_3$$
$$= -\frac{1}{\sinh\frac{cL}{\ell}}\left[\left(\cosh\frac{cL}{\ell} - 1\right)A_2 + \frac{\ell\phi'_L}{c}\right]. \tag{91}$$

Eqs. (87)–(90) become

$$\frac{T^{SV}(z)}{FL} = Z - \frac{\alpha_0 S}{c^2 AL}, \quad \frac{T^{\omega}(z)}{FL} = -c^2 Z,$$
$$\frac{T^{\text{pretwist}}(z)}{FL} = -(1-c^2)Z + \frac{\alpha_0 S}{c^2 AL}, \tag{92}$$

where

$$Z = \frac{1}{\sinh\frac{cL}{\ell}}\left\{\frac{GJ\phi'_L}{FL}\sinh\frac{cz}{\ell} + \frac{\alpha_0 S}{c^2 AL}\left[\sinh\frac{c(L-z)}{\ell} + \sinh\frac{cz}{\ell}\right]\right\}$$

and

$$\frac{B(z)}{FL^2} = \frac{1}{\sinh\frac{cL}{\ell}}\left\{\frac{1}{c}\frac{S}{AL^2}\left[\ell\alpha_0\cosh\frac{c(L-z)}{\ell} - \frac{\alpha_0^3 R}{cJ}\frac{E}{G}\sinh\frac{c(L-z)}{\ell}\right]\right.$$
$$\left. -\left(\frac{1}{c^2}\frac{S}{AL^2} + \ell\phi'_L\frac{GJ}{FL^2}\right)\left(\cosh\frac{cz}{\ell} + \frac{\alpha_0^2 R}{\ell J}\frac{E}{G}\sinh\frac{cz}{\ell}\right) + \frac{\alpha_0^3 R}{c^2 J}\frac{E}{G}\frac{S}{AL^2}\sinh\frac{cL}{\ell}\right\}. \tag{93}$$

The rotation of the cross section at the end $z = L$ is

$$\phi_L \equiv \phi(L) = \frac{\ell\phi'_L}{c}\tanh\frac{cL}{2\ell} - \frac{\alpha_0 SL}{J_{\text{eff}}}\frac{F}{GA}\left(1 - \frac{2\ell}{cL}\tanh\frac{cL}{2\ell}\right)$$
$$\simeq \frac{\ell\phi'_L}{c} - \frac{\alpha_0 SL}{J_{\text{eff}}}\frac{F}{GA}\left(1 - \frac{2\ell}{cL}\right), \tag{94}$$

where we took into account that $\ell/L \ll 1$ and $c = O(1)$. The above equation can written also in the form

$$\frac{F}{GA} = \frac{J_{\text{eff}}}{S}\frac{\frac{\ell}{cL}\frac{\phi'_L}{\alpha_0}\tanh\frac{cL}{2\ell} - \frac{\phi_L}{\alpha_0 L}}{1 - \frac{2\ell}{cL}\tanh\frac{cL}{2\ell}} \simeq \frac{c^2 J}{S}\left[-\frac{\phi_L}{\alpha_0 L} + \left(\frac{\phi'_L}{\alpha_0} - 2\frac{\phi_L}{\alpha_0 L}\right)\frac{\ell}{cL}\right]. \tag{95}$$

Define complete unwinding as: $\phi_L = -\phi_0(L) = -\alpha_0 L$ and $\phi\prime_L = -\alpha_0$. The required force F_{un} results from (95):

$$\frac{F_{un}}{GA} = \frac{J_{\text{eff}}}{S}\frac{1 - \frac{\ell}{cL}\tanh\frac{cL}{2\ell}}{1 - 2\frac{\ell}{cL}\tanh\frac{cL}{2\ell}} \simeq \frac{c^2 J}{S}\left(1 + \frac{\ell}{cL}\right). \tag{96}$$

We observe that F_{un} increases with increasing ℓ, i.e., the largest the characteristic length ℓ of the DNA beam, the stiffer the response. This is a new result and differs from the classic prediction of constant torsion stiffness of DNA that is based on the assumption of circular cross section.

As $\ell \to 0$, the unwinding force F_{un} approaches the limiting value of $\frac{c^2 J}{S}GA$. Eq. (96) shows that

$$F_{un} \geqslant \frac{c^2 J}{S}GA, \tag{97}$$

i.e., the unwinding force has a definite lower limit that depends on the geometry of the cross section and the shear modulus of the material.

Typical values for the DNA are $L = 35$ nm, $\alpha_0 = 0.04$ rad/nm $= 2.29^{\circ}$/nm (Bao, 2002). As mentioned in the introduction, a double-helical DNA chain has ten base pairs per helical turn of length 3.4 nm, i.e., $10a = 3.4$ nm, where a is the length of one base pair (Bao, 2002). Therefore, the initial twist rate of $\alpha_0 = 0.04\ \text{nm}^{-1} = 2.29^{\circ}\ \text{nm}^{-1}$ corresponds to an "excess linking number" of $\alpha_0 \times 10a = (0.04\ \text{nm}^{-1}) \times (3.4\ \text{nm}) = 0.136$. The resulting value from (96) for the unwinding force is

$$F_{un} \cong 92\ \text{pN}. \tag{98}$$

This estimate for F_{un} is higher than the transition value of $F_0 \cong 10$ pN mentioned in the Introduction, consistent with the assumption of entropic elasticity.

We conclude this section with a brief discussion of the effects of the material length ℓ on the solution. In the case of the DNA consider above the characteristic length of $\ell \simeq 0.5$ nm is small compared to its length of $L = 35$ nm and the effect of pretwist on torsional constant is negligible:

$$\frac{\ell}{L} \cong \frac{1}{70}, \quad c \cong 1, \quad J_{\text{eff}} \cong J. \tag{99}$$

This may not always be the case. For example, experiments with much smaller DNA lengths could be designed so that $\frac{\ell}{L} \cong \frac{1}{10}$ (Lee et al., 1994).

The size of ℓ controls the magnitude of the bimoment B and the part of the torque T^{ω} (both B and T^{ω} vanish in the classical case with $\ell = 0$). In the problem under consideration the total torque T vanishes; however, the individual components T^{SV}, T^{ω}, and T^{pretwist} are different from zero and satisfy the condition

$$T^{SV} + T^{\omega} + T^{\text{pretwist}} = 0 \tag{100}$$

everywhere along the DNA. The variation of the normalized components of the torsional moment and the normalized bimoment along the beam are shown in Figs. 8 and 9.

Figs. 8 and 9 show that the effects of "constrained warping" (or the "length scale effects") are limited to a region of about $0.05L \cong 3.5\ell$ at the fixed end of the DNA, i.e., the region over which T^{ω} and B take substantial values is about 3.5ℓ. Along the rest of the beam, T^{ω} and B essentially vanish and the Saint–Venant torque counteracts the pretwist $\left(T^{SV} \cong -T^{\text{pretwist}}\right)$.

5. Strength consideration for locally denatured DNA

Experiments indicate that the DNA strands can sustain very high stresses and that the DNA could fail due to excessive shearing of the weakest hydrogen bonds that hold the DNA strands together (Smith et al., 1992). Lee et al. (1994) used the atomic force microscope in order to measure the tensile rupture force of DNA molecules. In particular, 10 active DNA molecules were immobilized within the probe contact area of the microscope and the corresponding rupture force was measured. The reported values are in the range of 0.83 – 1.52 nN, with most of the values being between 0.83 and 1.3 nN (Lee et al., 1994). We can distribute this force to the average area of 10 molecules and calculate the average critical shear stress τ_{cr} that ruptures the bonding of the strands as

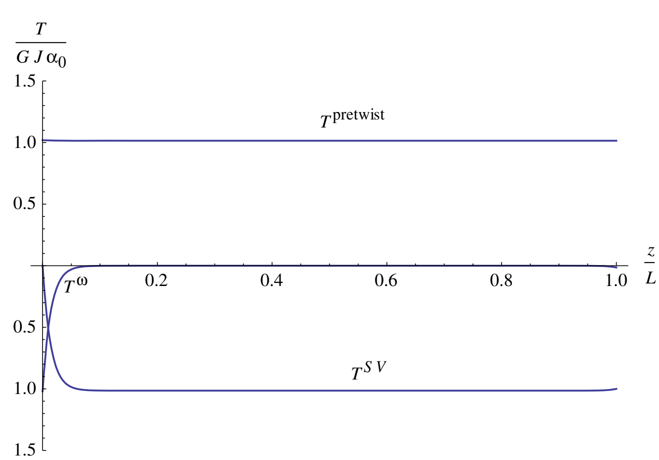

Fig. 8. Normalized torque distribution along the DNA. Note that $T^{SV} + T^{\omega} + T^{\text{pretwist}} = 0$ everywhere along the beam.

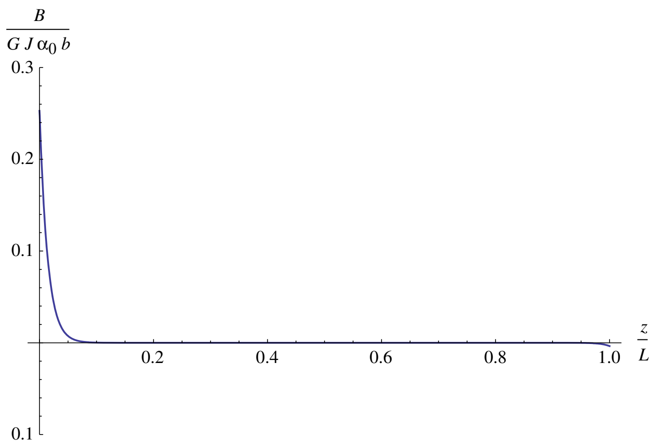

Fig. 9. Normalized bimoment distribution along the DNA.

$$\tau_{cr} = \frac{1}{2}\frac{F}{10bt} = \frac{1}{2}\frac{0.83 \text{ to } 1.3 \text{ nN}}{10 \times (2 \text{ nm}) \times (0.5 \text{ nm})} = 41.5 \text{ to } 65 \text{ MPa}. \tag{101}$$

At the full unwinding load of $F_{un} \cong 92$ pN the axial stress is

$$\sigma_{zz}^{un} = \frac{F_{un}}{bt} \cong \frac{92 \text{ nN}}{(2 \text{ nm}) \times (0.5 \text{ nm})} = 92 \text{ MPa}. \tag{102}$$

The maximum shear stress at the critical load is

$$\tau_{\max} = \frac{\sigma_{zz}^{un}}{2} \cong 46 \text{ MPa}, \tag{103}$$

which is close to the calculated shear strength. These results suggest that as complete unwinding of the DNA is approached, damage will commence, in good accord with experiments.

6. Conclusions

We have shown that the general problem of non-uniform torsion of thin-walled open cross section beams can be modeled with a strain gradient elasticity model. The general solution of the problem depends on classic boundary conditions and on non-classic conditions like the axial variation of the twist and the warping double torsion moment. Moreover, additional shear stresses develop due to the warping constrain which can have a pronounced effect on the strength of the beam. Self-equilibrated axial stresses develop in the beam and consequently an applied axial force can give rise to torsion of the beam due to the axial variation of the twist that develops in the structure. Thus, the analysis provides a coupling effect between the twist rate and the average axial strain of the cross section.

We have examined the tension of DNA at the stage that it unwinds completely and is almost straight. At tensile axial loads that are high enough, enthalpic elasticity becomes dominant. A key aspect of the analysis lies in the assumed shape of the DNA that resembles to a thin strip rather than a cylindrical rod.

A characteristic length appears in the problem formulation and is a fraction of the size of the cross section. As a result, a size effect appears naturally in the context of the present analysis and implies that shorter beams are stiffer in torsion than longer beams. Interestingly, Vlasov's theory of thin-walled, open cross section beams is identical to the presented gradient type of elasticity theory, with a characteristic length that depends inversely to the thickness of the section walls. The internal length that is predicted from the gradient elastic torsion model of DNA is about 0.5 nm. This leads to a stiffer response of DNA in torsion than what has been previously considered. The torsion response can be sensitive to the boundary conditions applied at the ends of the DNA molecule, especially when a short part of it is in tension.

Due to the initial pre-twist, the axial force that is required to straighten the DNA molecule gives high shear stresses that disrupt the bonding of the base pairs and separates the DNA strands. This critical shear stress is of order 46 MPa and can be produced by an axial force of the order of 92 pN. This load is of the same magnitude as the load that produces complete unwinding of the DNA, in good accord with available experimental measurements. An important conclusion of this work is that the complete unwinding of the DNA triggers its denature and debonding.

References

Bao, G., 2002. Mechanics of biomolecules. J. Mech. Phys. Solids 50, 2237–2274.
Baumann, C.G., Smith, S.B., Bloomfield, V.A., Bustamante, C., 1997. Ionic effects on the elasticity of single DNA molecules. Proc. Nat. Acad. Sci. U.S.A. 94, 6185–6190.
Bleustein, J.L., 1967. A note on the boundary conditions of Toupin's strain-gradient theory. Int. J. Solids Struct. 3, 1053–1057.
Chen, W-F., Atsuta, T., 2007. Theory of Beam-Columns, Volume 2: Space Behavior and Design. J. Ross Publishing.
Cluzel, P., Lebrun, A., Heller, C., Lavery, R., Viory, J.L., Chatenay, D., Caron, F., 1996. DNA: an extensible molecule. Science 271, 792–794.
Cook, R.D., Young, W.C., 1985. Advanced Mechanics of Materials. Macmillan Publishing Company, N.Y.
Corradi Dell'Acqua, L., 1992. Meccanica delle Struture, vol. I. McGraw-Hill Libri Italia.
Costello, G.A., 1983. Stresses in multilayered cables. J. Energy Res. Technol. Trans. ASME 105, 337–340.
Georgiadis, H.G., 2003. The mode-III crack problem in microstructured solids governed by dipolar gradient elasticity: static and dynamic analysis. J. Appl. Mech. 70, 517–530.
Georgiadis, H.G., Anagnostou, D.C., 2008. Problems of the Flamant–Boussinesq and Kelvin type in dipolar gradient elasticity. J. Elasticity 90, 71–98.
Georgiadis, H.G., Vardoulakis, I., Velgaki, E.G., 2004. Dispersive Rayleigh-wave propagation in microstructured solids characterized by dipolar gradient elasticity. J. Elasticity 74, 17–45.
Green, E., Rivlin, R.S., 1964. Multipolar continuum mechanics. Arch. Ration. Mech. Anal. 17, 113–147.
Goodier, J.N., 1962. Torsion. In: Flügge, W. (Ed.), Handbook of Engineering Mechanics. McGraw-Hill Book Company, Inc.
Hardy, G., Littlewood, J.E., Pólya, G., 1952. Inequalities, 2nd ed. Cambridge University Press.
Lazar, M., Maugin, G.A., 2005. Nonsingular stress and strain fields of dislocations and disclinations in first strain gradient elasticity. Int. J. Eng. Sci. 43, 1157–1184.
Lee, G.U., Chrisey, L.A., Colton, B.J., 1994. Direct measurement of the forces between complementary strands of DNA. Science 266, 771–773.
Librescu, L., Song, O., 2006. Thin-walled composite beams. Springer, The Netherlands.
Marko, J.F., 1997. Stretching must twist DNA. Europhy. Lett. 38, 183–188.
Mindlin, R.D., 1964. Microstructure in linear elasticity. Arch. Ration. Mech. Anal. 16, 51–78.
Oden, J.T., Ripperger, E.A., 1981. Mechanics of Elastic Structures, 2nd ed. Hemisphere Publishing Co.
Odijk, T., 1995. Stiff chains and fillaments under tension. Macromolecules 28, 7016–7018.
Papargyri-Beskou, S., Tsepoura, K.G., Polyzos, D., Beskos, D.E., 2003. Bending and stability analysis of gradient elastic beams. Int. J. Solids Struct. 40, 385–400.
Papargyri-Beskou, S., Polyzos, D., Beskos, D.E., 2009. Wave dispersion in gradient elastic solids and structures: A unified treatment. Int. J. Solids Struct. 46, 3751–3759.
Rosen, A., 1978. The effect of initial twist on the torsional rigidity of beams – Another point of view, Technion – Israel Institute of Technology, Department of Aeronautical Engineering, TAE, Report No. 360, Apr. 1978.
Rosen, A., 1980. The effect of initial twist on the torsional rigidity of beams – another point of view. J. Appl. Mech. 47, 483–515.
Rosen, A., 1991. Structural and dynamic behavior of pretwisted rods and beans. Appl. Mech. Rev. 44, 389–392.
Rees, D.W.A., 2000. Mechanics of Solids and Structures. Imperial College Press, New York.
Rodríguez, J.M., Viaño, J.M., 1993. Analyse asymptotique de l'équation de Poisson dans un domaine mince. Application à la théorie de torsion des poutres elastiques à profil mince. I. Domaine "sans jonctions". C.R. Sci. Paris, Série I 317, 423–428.
Shi, M.X., Huang, Y., Hwang, K.C., 2000. Fracture in the high-order elastic continuum. J. Mech. Phys. Solids 48, 2513–2538.
Smith, S.B., Finzi, L., Bustamante, C., 1992. Direct mechanical measurements of the elasticity of single DNA molecule by using magnetic beads. Science 258, 1122–1126.

Sokolnikoff, I.S., 1956. Mathematical Theory of Elasticity,, McGraw-Hill (reprinted by Robert E. Krieger Publishing Company, 1986).
Timoshenko, S.P., Gere, J.M., 1961. Theory of Elastic Stability. McGraw-Hill, N.Y.
Toupin, R.A., 1962. Elastic materials with couple-stresses. Arch. Ration. Mech. Anal. 11, 385–414.
Van Dyke, M., 1975. Perturbation Methods in Fluid Mechanics. The Parabolic Press, Stanford, CA.
Vardoulakis, I., Giannakopoulos, A.E., 2006. An example of double forces taken from structural analysis. Int. J. Solids Struct. 43, 4047–4062.
Vlasov, V.Z., 1969. Thin-Walled Elastic Beams, 2nd ed. (revised and augmented, translated from Russian and published for the National Science Foundation, Washington, D.C. and the Department of Commerce, U.S.A. by the Israel Program for Scientific Translations, Jerusalem).
Wagner, H., 1936. Torsion and buckling of open sections, National Advisory Committee for Aeronautics (NACA), Technical Memorandum No. 807 (English translation of Verdrehung und Knickung von offenen Profilen, from the 25th Anniversary Number of the Technische Hochschule Danzing, 1904–1929, pp. 329–343).