A broad range of fibers are found in biological materials, including collagen, elastin, fibrin, and smaller filaments such as F-actin, microtubules, and amyloids. Cellulose fibers, either extracted from plants or produced by bacteria, are processed and used in artificial network materials such as paper products and textiles. Engineering nonwovens are generally made from polymeric fibers. Glass fibers are used for sound and thermal insulation. The mechanical behavior of several classes of fibers is presented in this chapter.

A distinction is made between fibers with thermal and athermal behavior. Fibers of a diameter sufficiently large such that thermal fluctuations play no role in their mechanics are considered athermal. Flexible filaments with small or vanishing bending stiffness are subjected to thermal fluctuations, and this has a significant impact on their mechanical behavior. These are considered thermal filaments. Semiflexible filaments which exhibit features specific to both of these categories are also important, since many protein networks are of this type. This chapter includes separate discussions of these three fiber categories.

We recall here that the term “fiber” is used for athermal fibers, while “filament” is used for sub-micron fibers, whether of molecular or supra-molecular type.

In some materials, such as geotextiles and other nonwovens, the network is constructed from individual fibers. In some other cases, particularly in biological networks such as the extracellular matrix, the network is composed of filament bundles, where a bundle contains multiple filaments. The mechanical behavior of a bundle depends not only on the properties of the constituent fibers, but also on the way these are bonded together. A bundle in which fibers are weakly connected behaves differently from one in which fiber-to-fiber interfaces are strong. Fiber bundles have more complex mechanical behavior than individual fibers and this is reflected in the network-scale behavior. The mechanical behavior of bundles is discussed in Section 2.5.

2.1 Examples of Fibers and Fiber Properties

The mechanical behavior of fibers depends on their chemical composition and structure and is probed experimentally either in bending or tension. Variability from fiber to fiber is generally large and experiments can only provide ranges for the constitutive parameters. This section reviews fibers encountered in some of the most important current network materials: cellulose fibers, polymeric fibers, and collagen.
2.1.1 Cellulose Fibers

Cellulose is a polysaccharide which consists of D-glucose units linked in linear chains (Figure 2.1(a)). The chains are arranged in crystals stabilized by strong H-bonds established between the hydroxyl groups of neighboring molecules. This parallel molecular arrangement and the high density of intermolecular bonds convey high strength and stiffness to the crystal. The crystal strength increases as the chain length increases. Cellulose is semicrystalline, that is, it contains both crystalline and amorphous sub-domains. The fraction of the crystalline component varies greatly between plant species and is controlled during the subsequent chemical processing of the plant-derived material.

Cellulose is abundant in nature as it is the building block of the load-carrying structure of most plants. It represents 90% of the cotton and about 50% of the wood structure. Natural fibers contain lignin and hemicellulose in addition to cellulose. Hemicellulose is mostly amorphous and contains a variety of sugar monomers and imperfections which prevent the growth of crystals. This makes it less stiff than cellulose and more prone to hydrolysis by dilute acids. Lignin has a complex, disordered molecular structure which prevents crystallization.

Fibrils containing many molecular strands assemble to form fibers of larger than micrometer cross-sectional dimensions and complex structure. Fibers have successive layers, somewhat similar to the growth rings in wood. Cotton and wood-derived cellulosic fibers used to make paper are tubular, in the sense that they present a lumen, which typically collapses during drying such that the resulting fiber cross-section appears ribbon-like (Figure 2.1(b)). The arrangement of fibrils in the various layers of the fiber influences the fiber mechanical properties. The layers providing the mechanical function have fibrils that spiral around the axis of the fiber (Lichtenegger et al., 1999). Layer S2 in Figure 2.1(b) accounts for about 86% of the thickness of the tubular fiber wall and has cellulose fibrils oriented at an angle relative to the fiber axis. The outer layer denoted by P has a random fibril structure, while the thin layer S1 has fibrils oriented at a large angle (about 80°) to the fiber axis (Neagu et al., 2006). The helix angle defines the stiffness and the deformability of the fiber. This aspect of the

![Figure 2.1](https://doi.org/10.1017/9781108779920.003) Published online by Cambridge University Press
mechanics is discussed in Section 2.5.2.2. Here it suffices to indicate the rather obvious fact that a smaller angle (indicating strong alignment in the fiber direction) corresponds to stiffer fibers that deform less before breaking. Controlling the helix angle is an important mechanism by which the plant controls its stiffness. For example, fibril orientation varies greatly in a tree branch leading to a functionally graded material across the cross-section and along the branch, from the tree trunk to the outer extremity of the branch (Farber et al., 2001). The gradient changes spatially, depending on the local mechanical loading, so as to maximize flexibility while retaining strength.

The length of cellulose fibrils and fibers varies greatly as a function of their biological origin and the chemo-mechanical treatment to which they were subjected during processing. Cotton fibers have a length of the order of 3–4 cm, wool fibers range from a few centimeters to tens of centimeters and fibers in pulp and paper have lengths of 0.5–3 mm. Processes such as acid treatment and pulp beating reduce the fiber length and may modify the structure of the fiber wall. The cross-section characteristic dimension of these fibers is of tens of micrometers, such that typical aspect ratios for cotton and flax fibers are \( \sim 1500 \), while the aspect ratio of wool fibers is \( \sim 3000 \).

The mechanical properties of natural fibers also vary broadly as a function of the same factors that control the fiber length and as a function of the hydration state. Broad ranges of values for the modulus and strength of cellulose fibers are listed in Table 2.1. The properties of individual wood and pulp fibers used in paper depend on the state of hydration; a fiber wall thickness of 4 \( \mu \)m, fiber width (largest dimension of the cross-section) of 15–30 \( \mu \)m, and axial Young’s modulus of 35 GPa are typical values reported in the literature.

<table>
<thead>
<tr>
<th>Fiber Type</th>
<th>Characteristic Cross-section Dimensions (( \mu )m)</th>
<th>Young’s Modulus, ( E_f ) (GPa)</th>
<th>Strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural fibers</td>
<td>Cotton 10–20</td>
<td>1.5–3</td>
<td>150–400</td>
</tr>
<tr>
<td></td>
<td>Wool 15–40</td>
<td>2–3.9</td>
<td>120–180</td>
</tr>
<tr>
<td></td>
<td>Jute ( \sim 100 )</td>
<td>20–30</td>
<td>200–350</td>
</tr>
<tr>
<td></td>
<td>Rayon 12–40</td>
<td>0.5–1</td>
<td>100–250</td>
</tr>
<tr>
<td></td>
<td>Softwood 20–70</td>
<td>20–40</td>
<td>100–300</td>
</tr>
<tr>
<td>Synthetic polymeric fibers</td>
<td>Nylon ( \sim 20 )</td>
<td>5</td>
<td>( \sim 900 )</td>
</tr>
<tr>
<td></td>
<td>Aramid ( \sim 10 )</td>
<td>60–100</td>
<td>2000–3000</td>
</tr>
<tr>
<td></td>
<td>Polyester 10–50</td>
<td>15–20</td>
<td>300–1000</td>
</tr>
<tr>
<td></td>
<td>Polypropylene 20–50</td>
<td>3–5</td>
<td>200–700</td>
</tr>
<tr>
<td></td>
<td>Polyethylene (high molecular weight) 20–50</td>
<td>5</td>
<td>300–500</td>
</tr>
<tr>
<td>Other fibers</td>
<td>Glass 10–20</td>
<td>70–80</td>
<td>1400–4000</td>
</tr>
<tr>
<td></td>
<td>Carbon ( \sim 10 )</td>
<td>230–380</td>
<td>1800–2600</td>
</tr>
</tbody>
</table>

Note: See a collection of properties of various types of fibers in Mohanty et al. (2000).
2.1.2 Polymeric Fibers

Most artificial fibers made today are polymeric. Polymer viscosity in the melt state is a function of temperature, molecular weight (chain length), and the presence of solvents. This allows us to produce fibers of various diameters, from \( \sim 100 \) nm to hundreds of microns.

The most common fiber manufacturing process is spinning from the melt. This entails forcing the melt through a spinneret by applying pressure and/or suction on the opposite side of the melt bath. Fibers solidify during the flight time between the spinneret and the conveyor belt on which the fibrous mat is deposited. This procedure is used industrially to produce nonwovens and leads to fibers with typical diameter of tens of microns (Figure 2.2). Note that textile fibers also have diameters of tens of microns, while the diameter of a human hair is of the same magnitude (20–50 \( \mu \)m).

Electrospinning is a newer process which was developed to produce polymeric fibers of sub-micron diameter. This method is similar to spinning, but allows drawing the fiber during its flight time, after the fiber forms at the spinneret, by the application of an electric field. The flow undergoes an instability that leads to a substantial reduction of the diameter. The mechanics of spinning and electrospinning are described in a large number of articles (e.g., McHugh and Doufas, 2001) and summarized in recent texts (e.g., Andrady, 2008).

The most common polymers used in fiber production are polypropylene and polyethylene, which are broadly used in nonwovens of various types, and nylon, polyester, and acrylic, which are used in textiles. Fibers are made from other synthetic polymers as well, such as polyurethane and aromatic polyamides (aramids). Polymeric fibers can be spun as single components or as core-shell and side-by-side composite fibers made from two constituents. The side-by-side fibers may be spun with a helical geometry.

![Image](https://doi.org/10.1017/9781108779920.003 Published online by Cambridge University Press)
Fibers made from natural polymers which are chemically decomposed and reconstituted may be produced. The earliest example of this type is rayon (viscose and modal are specific types of rayon), which is obtained from purified cellulose extracted chemically from wood pulp. Cellulose diacetate and cellulose triacetate are obtained by chemically treating cellulose with acetic acid or acetate esters, which preserves the glucose backbone of cellulose (Figure 2.1(a)), but add two and three, respectively, acetate groups to the ring. Fibers are currently being produced from reconstituted collagen, which can be spun in mats supposed to mimic the extracellular matrix and used as scaffolds for tissue engineering. The properties of reconstituted collagen depend on the temperature at which synthesis takes place.

Polymer spinning causes strong uniaxial stretching of the melt, which leads to preferential chain orientation in the flow direction. The alignment favors polymer crystallization. In strong flows, new polymer structures form; an example is the shish-kebab structure composed of a strongly aligned bundle of polymeric chains (the shish) on which disc-like crystalline lamellae form in the direction perpendicular to the fiber direction (the kebab). Such strong alignment and, in particular, the partial crystallization, impart high stiffness and high strength to the fibers, which are highly desirable properties in most applications. In addition, the surfaces of spun and electrospun fibers are generally quite smooth (Figure 2.2(a)), with roughness well below the micron range, which increases the strength of fibers.

Spun polymeric fibers are of “infinite length,” which is a result of the continuous nature of the spinning process. When deposited in mat form, fibers are tortuous and have random orientations. Preferential fiber orientations may be obtained by depositing on a spinning mandrel.

The properties of synthetic polymeric fibers depend on the type of polymer and processing method used and have less variability than those of natural fibers. An example of the mechanical response in uniaxial tension of an iPP (isotactic polypropylene) fiber similar to that in Figure 2.2(a) is shown in Figure 2.2(b). The three curves correspond to fibers processed at take-up velocities of 1 000, 2 000, and 3 000 m/min (Osta et al., 2014). Increasing the take-up velocity (i.e., the velocity at which the fiber exits the spinneret) increases chain alignment, the yield stress, and the strength. Richaud et al. (2009) report that increasing the draw ratio of iPP fibers from 4 to 10 increases the modulus from 3 to 15 GPa and the strength from 200 to 600 MPa. Typical values of the stiffness and strength of some common polymeric fibers are reported in Table 2.1.

### 2.1.3 Collagen

Collagen fibers play an essential mechanical role in tissues of invertebrate and vertebrate organisms. In the human body collagen is present in the extracellular matrix, in connective tissue such as cartilage and tendons, in various membranes and blood vessels and, as mineralized collagen, in bones. Multiple types of collagen exist, of which types I to V are the most prevalent, with some being present only in specific tissues. Type I collagen, which is one of the fibrillar collagen types, is the
most abundant in the body, being present in tendons, skin/dermis, and arterial walls. Type II, which is also of fibrillar type, is the main component of cartilage.

Collagen has a hierarchical, multiscale structure (Figure 2.3). The present discussion is focused on the structure of fibrillar collagen. The building block is tropocollagen (Figure 2.3(a)), which is a right-handed helix made from three polypeptide molecules. This structure was recently imaged in three-dimensions (Orgel et al., 2001). On the next hierarchical level, tropocollagen molecules of ~300 nm length assemble to form collagen fibrils. The axial arrangement of tropocollagen in the fibril is staggered, that is, tropocollagen strands are arranged in a sequence along the axial direction of the fibril, with gaps between each other, while the gaps of neighboring rows of strands are not aligned (Figure 2.3(b)). The three-dimensional arrangement is complex and it is currently considered that, in the cross-section, the strands have a semi-ordered quasi-hexagonal arrangement, as indicated in Figure 2.3(c) (Orgel et al., 2001). In the simplified view of the axial arrangement shown in Figure 2.3(b) it is

Figure 2.3 Schematic representations of (a) tropocollagen and (b) fibrils showing the characteristic staggering of tropocollagen molecules (reprinted from Sherman et al. (2015) with permission from Elsevier). (c) Arrangement of molecules in the cross-section view of the fibril in (b) (reprinted from Orgel et al. (2001), with permission from Elsevier). (d) Image of fibril bundle forming a fiber (reprinted from Sherman et al. (2015), with permission from Elsevier). The D-band staggering indicated in (b) is visible in this image. (e) Stress–stretch curves of a reconstituted collagen fibril of ~300 nm diameter (data from Liu et al., 2018), and of a reconstituted collagen fiber of ~50 μm diameter (data from Sopakayang et al., 2012). As the diameter increases, fibers with hierarchical structure have lower load carrying capacity.
suggested that staggering involves a shift of ~67 nm, the so-called D-period, which represents approximately a quarter of the tropocollagen length. The axial gap size is 0.54 of the D-period. When imaged in the direction perpendicular to the fibril axis, a clear periodicity associated with this staggering is observed (Figure 2.3(d)). The diameter of a typical fibril is of about 100–200 nm.

Neighboring tropocollagen strands are connected by enzymatic and nonenzymatic crosslinks which ensure the load transfer between fibrils. Enzymatic crosslinking occurs predominantly at the ends of the tropocollagen strands. Nonenzymatic cross-links due to glycation occur more randomly along the strands and lead to substantial stiffening and associated pathologies.

On the next level of the hierarchy, fibrils form bundles and fibers of diameter on the order of microns and larger. The extracellular matrix and connective tissue are composed from such fibers whose fibril bundles split and merge with neighboring fibers to create a stochastic network (Figure 1.1(d)).

The mechanical properties of collagen are of much interest in biomechanics and have been investigated by many groups. A review is available in Sherman et al. (2015). The effective stiffness of tropocollagen measured on the molecular scale by monitoring thermal fluctuations leading to the evaluation of the persistence length is reported to range from 3 to 4 GPa. Direct stretching of fibrils provides values between 400 and 800 MPa. Testing fibers of above micrometer diameters leads to a broad range of values which depend on the hydration state, degree of tortuosity, and the origin of the respective fiber. The stiffness of the building blocks is larger than that of the larger scale collagen structures, as predicted by the mechanics of discontinuous fiber bundles discussed in Section 2.5.3. Figure 2.3(e) shows stress–strain curves obtained by uniaxial stretching individual collagen fibrils (Liu et al., 2018) and fibers (Sopakayang et al., 2012).

### 2.2 Energetic and Entropic Mechanical Behavior

Before discussing the mechanical behavior of fibers and networks, it is necessary to clarify the origin of stress in these systems.

Consider a classical system described in terms of a set of kinematic parameters, $\mathbf{A}$, and the absolute temperature, $T$. In the canonical ensemble, the representative thermodynamic potential is the Helmholtz free energy:

$$\Psi(\mathbf{A}, T) = U(\mathbf{A}, T) - T\Sigma(\mathbf{A}, T),$$  \hspace{1cm} (2.1)

where $U$ and $\Sigma$ are the internal energy and the entropy of the system. The free energy is related to the partition function, $Z(\mathbf{A}, T)$, through the relation

$$\Psi(\mathbf{A}, T) = -k_B T \log Z(\mathbf{A}, T).$$

If the system is perturbed by an externally-imposed strain, $\varepsilon$, at least one member of the kinematic parameter set $\mathbf{A}$, $\mathbf{A}_i$, varies with the applied strain, that is, $\partial \mathbf{A}_i / \partial \varepsilon \neq 0$. Then, the quantity
\[ \sigma = \frac{\partial \Psi}{\partial \varepsilon} = \frac{\partial \Psi}{\partial \mathcal{A}_i} \frac{\partial \mathcal{A}_i}{\partial \varepsilon} \]  
(2.2)

is the stress, work conjugate with the prescribed strain.

With Eq. (2.1), one may rewrite the stress as:

\[ \sigma = \frac{\partial \Psi}{\partial \varepsilon} = \frac{\partial U}{\partial \varepsilon} - T \frac{\partial \Sigma}{\partial \varepsilon} = \sigma_U + \sigma_\Sigma, \]  
(2.3)

where the derivatives are evaluated at constant temperature and number of atoms. Equation (2.3) indicates that stress has two components in this ensemble: one related to the variation of the system energy, \( \sigma_U \), and the other related to the variation of the entropy, \( \sigma_\Sigma \), during deformation.

Since the entropy is given by \( \Sigma = -\partial \Psi/\partial T \), it is possible to write \( \partial \Sigma/\partial \varepsilon = -\partial^2 \Psi/\partial \varepsilon \partial T = -\partial \sigma/\partial T \). Hence,

\[ \sigma_\Sigma = T \frac{\partial \sigma}{\partial T}. \]  
(2.4)

Consider a monatomic crystal lattice with no defects at zero Kelvin (static case; Figure 2.4(a)). The lattice exists in only one configuration that, in the absence of defect nucleation or amorphization, remains well-defined during the elastic deformation. Therefore, the entropy vanishes. The internal energy is defined by interactions occurring between atoms. Deformation leads to the variation of the internal energy, since the interatomic distances change with strain. The free energy variation is therefore equal to the variation of the internal energy and stress is purely energetic in this case.

Consider further a string composed of a large number of rigid links (Figure 2.4(b)). The links are pin-jointed and rotate freely relative to each other. Since the links are not deformable, the system stores no internal energy. On the other hand, for any end-to-end distance, the string may take a large number of configurations. This number is maximum when the two ends are co-located. As the string is stretched and the distance between its ends increases, the number of available configurations decreases. In the

Figure 2.4 Schematic representations of (a) a monatomic lattice, (b) a freely rotating string, and (c) a periodic lattice of “nodes” connected by strings.
limit of a straight string, only one configuration is available. Therefore, the entropy of
the string decreases continuously during stretching. The free energy of this system is
equal to its entropic component \( \Psi = -T \Sigma \), and stress is purely entropic.

These two examples are idealizations. In real systems both entropic and energetic
components are non-zero and in some cases one of the two components dominates.
A monatomic crystal develops defects during deformation and the defect density
increases with strain. The entropy of the system is not zero and increases as the crystal
deforms. At finite temperatures, lattice vibrations lead to another entropic component
of the free energy. The variation of the phonon spectrum with the strain is the physical
basis of the entropic component of the stress in perfect lattices. For a mathematical
description of this term, see Weiner (1983). However, the energetic component of
stress remains dominant in most monatomic crystalline solids.

In order to emphasize that the nature of stress depends on the state of the system,
consider an imaginary material which is a cross between the two examples discussed
in the previous three paragraphs: a periodic lattice of nodes which are connected by
strings (Figure 2.4(c)). The links of these strings are allowed to interact energetically
with other links which are not immediately bonded to them along the same string.
Deformation changes the end-to-end distance of most strings and the entropy of
the system. Therefore, the system has non-zero energy and entropy, and both components
of the free energy vary during deformation. Both entropic and energetic components
of the stress are non-zero. This idealized example is a proxy for rubber, which is a
crosslinked molecular network. However, another component of the physics is active
in rubber and this substantially modifies the physical picture. The links are quite
mobile since the material is above the glass transition temperature in ambient condi-
tions. This allows them to relax in configurations of minimum local energy on time
scales shorter than those of network deformation. As the system deforms, the local
environment of the links evolves, but these states are energetically equivalent since
packing does not change significantly. This implies that the energy of the system is
approximately constant during deformation and hence the energetic component of
stress is negligible. Although, in principle, the stress has both energetic and entropic
components, fast relaxation of the energetic component renders the system
approximately entropic.

This example helps in understanding another important characteristic of these
physical systems, which points to limitations of the applicability of the entropic stress
concept. A string must explore all configurations available to it at all times during
deformation in order to probe the variation of its entropy. This implies that (i) the
string should be sufficiently mobile to explore its phase space and (ii) the rate of the
imposed deformation should be such that the string is given sufficient time to perform
the sampling. If these conditions are not fulfilled, the entropy is constant during
deformation and the entropic component of stress vanishes.

Polymeric networks are typically considered thermal networks and stress is purely
entropic. However, if the deformation rate is high, the energetic stress component is
not relaxed effectively by local atomic scale processes and becomes non-negligible
relative to the entropic component. Furthermore, reducing the mobility by, for
example, reducing the temperature toward the glass transition temperature, reduces the ability of molecular strands to sample their phase space and reduces the importance of the entropic component relative to the energetic counterpart. Stress in polymeric networks below the glass transition temperature is energetic.

This discussion applies equally to individual fibers and to networks and provides the physical background for the distinction made here between thermal and athermal systems. The entropic component of stress is important in thermal networks, while athermal networks are purely energetic. Semiflexible filaments, in which both components are non-negligible, exhibit a richer behavior, which is discussed in Section 2.4.4.

2.3 Athermal Fibers

Athermal fibers have diameters sufficiently large for thermal fluctuations to play no role in their mechanics. Therefore, they can be treated as classical beams. Their elastic and inelastic behavior, stability, and strength are discussed in this section, with an eye on the aspects of the fiber behavior which are important for the mechanical response of the network.

2.3.1 Small Deformations

Beams store energy in the axial, bending, and torsion deformation modes. Under infinitesimal deformations these modes are independent, in the sense that the applied deformation corresponding to one mode does not do work against loads associated with other deformation modes. Energy storage caused by shear associated with transverse forces becomes important for beams of low aspect ratio (i.e., small cross-sectional dimensions relative to the axial length).

The geometric parameters characterizing fibers of circular cross-section are the fiber diameter, \( d \), and the fiber length, \( L_0 \). If the deformation is elastic, the only mechanical parameter of importance is the effective stiffness, which is defined as the ratio of the applied load to the conjugated measure of deformation. However, the effective stiffness depends on the boundary conditions. The loading configurations most relevant for networks of fibers are similar to those shown in Figure 2.5, with axial, bending and torsional loads acting at the ends of the fiber. Solutions for these

![Figure 2.5 Axial, bending, and torsional loading modes of straight beams.](https://doi.org/10.1017/9781108779920.003)
boundary value problems are obtained within the linearized beam theory which can be found in many texts (Gere and Timoshenko, 2002). The effective stiffness corresponding to each of these loading modes is listed in Table 2.2. \( E_f \) and \( G_f \) represent the Young’s and shear moduli of the fiber material, and \( A_f, I_f, \) and \( J_f \) represent the area, axial moment of inertia, and polar moment of inertia of the fiber cross-section relative to its centroidal principal axes, respectively. For the circular cross-section, \( A_f = \pi d^2 / 4, I_f = \pi d^4 / 64, \) and \( J_f = 2I_f = \pi d^4 / 32. \)

The Timoshenko model leads to the total strain energy of a beam:

\[
U = \frac{1}{2} \int E_f I_f \left( \frac{d\theta(s)}{ds} \right)^2 + E_f A_f \left( \frac{du(s)}{ds} \right)^2 + G_f J_f \left( \frac{d\varphi(s)}{ds} \right)^2 + \gamma G_f A_f \left( \frac{dw(s)}{ds} - \theta(s) \right)^2 \, ds. \tag{2.5}
\]

The integral is written in terms of \( s \), a curvilinear coordinate along the fiber, and is performed along the entire fiber length. The four terms represent the bending, axial, torsion, and shear energies, respectively. In this expression, \( \theta(s), \varphi(s), u(s), \) and \( w(s) \) represent the \( s \)-dependent rotation of a plane which remains perpendicular to the neutral axis of the fiber, the torsional rotation of a section about the neutral axis, axial and transverse displacements, respectively. \( \frac{dw(s)}{ds} - \theta(s) \) represents the additional rotation of the fiber cross-section due to shear. In the Timoshenko theory the cross-section of the beam is not perpendicular to the beam axis due to the shear loading. The Euler–Bernoulli model is a particular case of the Timoshenko model which neglects the contribution of shear. In this approximation, the last term in Eq. (2.5) is absent. Accounting for the contribution of the shear term is important for beams of small aspect ratio. As discussed in Chapter 4, the distribution of fiber segment lengths in random networks is of Poisson type (exponential) and hence many fibers segments are short. This suggests that the Timoshenko model is preferable to the Euler–Bernoulli model as a description of the mechanical behavior of athermal network fibers (Shahsavari and Picu, 2012).

In complex structures of beams, loading is such that multiple fiber deformation modes are enabled at the same time. The way the strain energy is distributed across these modes is defined by the effective stiffness of the structure. Figure 2.6(a) shows a beam loaded by a force \( P \) making an angle of \( \pi / 4 \) with the axis of the beam, such that the axial and bending modes are enabled by forces of equal magnitude. The energy stored in the axial mode is given by \( U_{ax} = P^2 L_0 / 4E_f A_f \), while the energy stored in the bending mode is \( U_{bd} = P^2 L_0^3 / 12E_f I_f \). The ratio of the two energies is \( U_{ax} / U_{bd} = (3/16)(d / L_0)^2 \ll 1. \) Hence, under load control, the fiber stores energy predominantly in the bending mode. Note that the ratio of the effective stiffnesses of

### Table 2.2 Effective stiffness of slender beams loaded as shown in Figure 2.5

<table>
<thead>
<tr>
<th>Loading Mode</th>
<th>Axial</th>
<th>Bending, Transverse Force</th>
<th>Bending, Bending Moment</th>
<th>Torsion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective stiffness ( p_1 )</td>
<td>( \frac{E_f A_f}{L_0} )</td>
<td>( \frac{3E_f I_f}{L_0^2} )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
</tr>
<tr>
<td>Effective stiffness ( p_2 )</td>
<td>( \frac{12E_f I_f}{L_0^3} )</td>
<td>( \frac{6E_f I_f}{L_0^3} )</td>
<td>( \frac{6E_f I_f}{L_0^3} )</td>
<td>( \frac{6E_f I_f}{L_0^3} )</td>
</tr>
<tr>
<td>Effective stiffness ( M_3 )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
<td>( \frac{E_f I_f}{L_0} )</td>
</tr>
<tr>
<td>Effective stiffness ( M_5 )</td>
<td>( \frac{G_f J_f}{L_0} )</td>
<td>( \frac{G_f J_f}{L_0} )</td>
<td>( \frac{G_f J_f}{L_0} )</td>
<td>( \frac{G_f J_f}{L_0} )</td>
</tr>
</tbody>
</table>

https://doi.org/10.1017/9781108779920.003 Published online by Cambridge University Press
the two modes (Table 2.2) is $k_{bd}/k_{ax} = (3/16)(d/L_0)^2$ in this particular case, that is, $U_{ax}/U_{bd} = k_{bd}/k_{ax}$, which implies that fibers store energy primarily in the softer deformation mode.

Consider now the equivalent displacement boundary value problem (Figure 2.6(b)). A displacement is applied at an angle $\pi/4$ relative to the fiber axis, such to equally activate the two deformation modes. In this case, the energy ratio is $U_{ax}/U_{bd} = (16/3)(L_0/d)^2 \gg 1$. Therefore, under displacement control, the fiber stores energy predominantly in the stiffer, axial mode.

In the load control case, the fiber behaves as if the two modes are connected in series. In displacement control, the two modes appear to be acting in parallel. Since one mode (axial) is much stiffer than the other, the apparent stiffness of the fiber is smaller under load control than when probed in displacement control.

A similar situation is encountered in composites made from stiff and soft phases. In this context, imposing an affine deformation, that is, forcing the two phases to deform by the same strain, leads to the upper bound of the composite stiffness. On the other hand, requiring that each phase carries the same load leads to the lower bound estimate for the effective composite stiffness. These are known as the Voigt and Reuss bounds, respectively. In Chapter 6 it is shown that the same applies on the scale of the network that, if forced to deform affinely, exhibits the largest attainable stiffness, while, if allowed to reduce its energy by nonaffine deformations, has a much lower stiffness.

### 2.3.2 Large Deformations

The linear beam theory cannot represent the geometric nonlinearity associated with large deformations. Beams undergo large deformations primarily in the bending mode. The geometric nonlinearity associated with large deformations was accounted for in the initial work on the mechanics of slender beams by Jacob Bernoulli (1654–1705), his nephew Daniel Bernoulli (1700–1782), and Leonard Euler (1707–1783). Jacob Bernoulli investigated the deformed shape of a beam loaded in bending and related the axial deformation of planes parallel to the neutral axial to the applied bending moment. Daniel Bernoulli correctly identified that the strain energy of a small segment of the beam is proportional to the square of the beam curvature at the respective site and suggested to Euler that his then new variational calculus can be used to find a solution for the beam deformation problem. Euler’s follow-up analysis led to the governing equation which reads:
\[ \kappa(x) = \frac{M}{E_f I_f}(x), \quad (2.6) \]

where \( \kappa(x) \) is the curvature of the beam at position \( x \) of the undeformed configuration, \( M \) is the applied bending moment in the same cross-section, and \( E_f I_f \) characterizes the beam material and the cross-section geometry. The left hand side of Eq. (2.6) may be written in terms of the deflection of the beam, measured in the direction perpendicular to the initial beam axis, \( w(x) \), as

\[ \frac{d^2w}{dx^2} = \frac{M}{E_f I_f}(x), \quad (2.7) \]

Equation (2.7) is a nonlinear differential equation for \( w \) and the nonlinearity is of geometric type. This expression can be linearized by neglecting \( dw/dx \) relative to 1 in the denominator. Since \( dw/dx = \tan \theta \), with \( \theta \) being the angle between the tangent unit vector and the undeformed beam axis, the respective approximation requires that the tangent slope of the beam is small. Within this approximation, Eq. (2.7) becomes:

\[ \frac{d^2w}{dx^2} = \frac{M}{E_f I_f}(x), \quad (2.8) \]

which can be readily integrated to derive the shape of the deformed beam, \( w(x) \), for given distribution of moments, \( M(x) \). The linearized formulation (2.8) is used to derive the results presented in Section 2.3.1 and Table 2.2.

Since the small deformation formulation (Eq. (2.8)) is entirely linearized, both geometrically and in terms of the beam material behavior, superposition applies. Solutions for complex loading situations can be obtained by superimposing solutions for simpler problems with same boundary conditions. This does not apply in nonlinear systems and, in such cases, Eq. (2.7) has to be solved for each loading and boundary condition separately.

Several features of the nonlinear beam bending problem are of importance for the broad understanding of network mechanics. We recall one of the best known and most relevant (in the context of networks) problems of this type: the bending of a cantilever beam by a concentrated force acting at its end (Mattisson, 1981; Fertis, 1999). Two possibilities are considered, with the force preserving its initial direction (Figure 2.7(a))

**Figure 2.7** Cantilever beam loaded by (a) a force preserving its initial direction and (b) a follower force.
and with the force remaining perpendicular to the beam axis, which is also known as the “follower force” problem (Figure 2.7(b)). Figure 2.8 shows the displacement of the point of application of the force in the two cases of Figure 2.7, and in the two directions, $x_1$ and $x_2$. The figure also shows the deflection (displacement in the direction perpendicular to the undeformed beam axis) computed with the small deformation formula (i.e., $\delta_2 = w(L_0) = PL_0^3/(3EI_f)$), and the axes are normalized such to render the small deformation solution a straight line. This emphasizes the difference between the linear and nonlinear solutions and shows the rapid change of the effective, instantaneous stiffness in the nonlinear case.

Figure 2.9 shows the tangent stiffness (derivative of the applied force with respect to the displacement $\delta_2$), versus the applied force computed from the data in Figure 2.8. The force is normalized with $3EI_f/L_0^2$ and $\delta_2$ is normalized with $L_0$, as in Figure 2.8. With this normalization, the small deformation formula gives a horizontal line at 1. The geometric nonlinear effect becomes pronounced for normalized forces.

![Figure 2.8](https://doi.org/10.1017/9781108779920.003)  
**Figure 2.8** Force-displacement relations for a cantilever beam loaded with a vertical force (Figure 2.7(a)) and a follower force which remains normal to the beam at all times (Figure 2.7(b)).

![Figure 2.9](https://doi.org/10.1017/9781108779920.003)  
**Figure 2.9** Normalized tangent stiffness versus normalized force for the curves in Figure 2.8.
$PL_0^2/3EI_f$ larger than 0.1, which corresponds to $\delta > 0.2L_0$. Beyond this threshold, the response becomes softer. The behavior shown in Figure 2.9 is also observed if the tangent stiffness is plotted versus $\delta/L_0$, that is, as if the beam would be loaded in displacement control.

A significant difference between displacement and load control is observed when investigating the increment of work performed (or stored strain energy) associated with an increment of the controlled variable. Under displacement control, the increments of work increase continuously as the beam response becomes stiffer. However, in load control, the increments of work decrease as the load increases.

Before closing this section, the geometrically exact beam formulations should be recalled. The first complete theory that eliminates the approximations of the Euler–Bernoulli theory and which accounts for large deformations and bending, axial, torsion, and shear deformation modes was developed by Reissner for two- and three-dimensional problems in 1972 (Reissner, 1972) and 1981 (Reissner, 1981), respectively. A large number of variants of this theory and the details of their numerical implementation, including the discussion of their objectivity and path dependence, have been published (e.g., Crisfield and Jelenic, 1999; Jelenic and Crisfield, 1999). A comparison of such models is presented in Romero (2008) and a historical perspective on their evolution is provided in Armero and Valverde (2012).

2.3.3 Relevance of Fiber Buckling for the Deformation of Fiber Networks

It is often claimed that fiber buckling takes place during the deformation of random networks and that this has important consequences on the overall network behavior. We indicate here that buckling instabilities of individual fibers are unlikely to occur. However, instabilities involving groups of fibers occur frequently.

Consider the loading shown in Figure 2.10(a) in which a compressive force, $P_{ax}$, loads the beam axially, along with a transverse force, $P = aP_{ax}$. If only the axial force is applied ($a = 0$), the Euler buckling problem is recovered. The critical buckling

![Figure 2.10](https://doi.org/10.1017/9781108779920.003) Published online by Cambridge University Press
force for these boundary conditions is \( P_{cr} = \pi^2 E_f I_f / 4 L_0^2 \). The deflection \( w(L_0)/L_0 \) for \( P_{ax} < P_{cr} \) is zero, but increases rapidly once the critical load is reached, as shown in Figure 2.10(b). The exact solution shown here is given in Bazant and Cedolin (2010). The increment of the axial force versus the increment of \( w(L_0)/L_0 \) immediately after the critical point is vanishingly small, that is, \( (P_{ax} - P_{cr}) / P_{cr} \approx \pi^2 / 8 (\delta_2 / L_0)^2 \). The incremental work performed by the axial force changes from being proportional to the square of the incremental axial strain \( u(L_0)/L_0 \) measured in the \( x_1 \) direction, when the beam deforms in the axial mode, to being approximately linear in \( u(L_0)/L_0 \) for \( P_{ax} > P_{cr} \), since the deformation after the instability takes place at essentially constant axial force.

The behavior of the beam changes drastically in the presence of a force acting perpendicular to the beam axis at the free end, \( P = aP_{ax} \). The deflection \( w(L_0)/L_0 \) is shown in Figure 2.10(b) for several non-zero values of \( a \). The instability is removed in the presence of the transverse force. A similar situation results when bending moments are applied in place of the transverse force and acting along with the axial force. This solution is presented in most books on structural stability (Timoshenko and Gere, 1961; Bazant and Cedolin, 2010) and resembles the curves shown in Figure 2.10(b) for \( a > 0 \).

If a torsion moment, \( M_1 \), is applied along with the axial compressive force, \( P_{ax} \), the situation is slightly more complicated but remains of buckling type. Solutions for various boundary conditions are presented in Bazant and Cedolin (2010). Here we confine attention to the boundary conditions that render the problem conservative: the beam is fixed at \( x_1 = 0 \), while the end at \( x_1 = L_0 \) is free to shift in the direction perpendicular to the undeformed beam axis, but it is prevented from rotating about axis \( x_2 \), \( w'(L_0) = 0 \). The critical conditions are described by the equation \( M_1^2 / 4 E_f I_f + P_{ax} = \pi^2 E_f I_f / L_0^2 \) (Timoshenko and Gere, 1961), where \( P_{ax} \) is positive in compression.\(^1\) Note that the presence of a torsion moment reduces the critical axial stress for the buckling instability.

In a random network, fibers are loaded in complex ways and it is extremely improbable that any fiber would be loaded exclusively with an axial force or axial moment. Therefore, buckling of individual fibers is largely irrelevant in networks, since the presence of loads other than axial removes the usual beam buckling instabilities.

However, instabilities that involve multiple fibers and are associated with local soft modes are frequent. The critical states for these instabilities cannot be estimated based on simple theoretical considerations due to the stochastic nature of the fiber arrangement and boundary conditions of the group of fibers that undergo the respective instability.

---

\(^1\) The Euler buckling critical load for the respective boundary conditions is recovered for \( M_1 = 0 \). The torsional moment acting alone (when \( P_{ax} = 0 \)) may produce buckling at a critical value given by this expression. The presence of a tensile axial force (\( P_{ax} < 0 \), in the notation of Figure 2.10(a)) increases the critical torsional buckling moment, and therefore stabilizes the beam.
2.3.4 Straight Fibers with Noncircular Cross-section

In many networks, fibers have a noncircular cross-section, and this introduces additional complexities. In some real networks, the cross-section is not even constant along any given fiber, with variability in the shape and size of the cross-section being sometimes pronounced, particularly in the case of natural fibers such as cellulose fibers in paper and cotton, flax, and other natural fibers used in textiles. Therefore, it becomes of interest to discuss the effect of the fiber cross-section shape on the mechanics of the network.

Any fiber cross-section has two principal axes of inertia. The principal axial moments of inertia, \( I_{\text{min}} \) and \( I_{\text{max}} \), are computed in terms of the section geometry and dimensions (Gere and Timoshenko, 2002). If the difference between these values is large, \( I_{\text{max}} \gg I_{\text{min}} \), and the fiber is loaded in bending in the stiffer mode, it becomes energetically favorable for the fiber to rotate and bend in the softer mode.

To demonstrate this effect, consider the cantilever beam shown in Figure 2.11(a), loaded by a force \( P \) acting in the \( x_2 \) direction. The beam has rectangular cross-section and is oriented with its longer edge along \( x_2 \), such that \( x_2 \) and \( x_3 \) are the principal axes of inertia and \( I_3 \gg I_2 \). As shown, the force bends the beam in the \( x_1 - x_2 \) plane (i.e., in the stiffer bending mode). However, it is more likely that the beam twists and bends in the softer mode, to reduce the stored strain energy, as shown schematically in Figure 2.11(b). This process is known as “lateral buckling.”

The critical load \( P_{\text{cr}} \) leading to lateral buckling is given by

\[
P_{\text{cr}} = \gamma^{**} \sqrt{E_f I_{\text{min}} K_t / L_0^2},
\]

where, for the configuration in Figure 2.11(a), \( I_{\text{min}} = h b^3 / 12 \), and \( K_t \) is the torsional rigidity of the beam given by \( K_t = \gamma^* G_f h b^3 \). \( G_f \) is the shear modulus and parameter \( \gamma^* \) is a function of the ratio \( \zeta = h / b \) which, for \( \zeta \geq 1.5 \), can be approximated with the function \( \gamma^* \approx \zeta^2 / \left[ 3 (\zeta + 0.4)^2 \right] \). Parameter \( \gamma^{**} \) is a slowly varying function of \( \zeta \), taking values of 4.013 for \( \zeta = 10 \) and 5.03 for \( \zeta = 3 \) (Timoshenko and Gere, 1961).

If the beam in Figure 2.11(a) is loaded in pure bending with a moment \( M \) aligned with axis \( x_3 \), lateral buckling sets in at a critical moment given by

\[
M_{\text{cr}} = \pi \sqrt{E_f I_{\text{min}} K_t / L_0},
\]

and, after this instability, the beam continues to bend in the softer mode characterized by the moment of inertia \( I_{\text{min}} (I_{\text{min}} = I_2 \) in Figure 2.11(a)).

The expression of the critical transverse force for lateral buckling may be rearranged as

\[
P_{\text{cr}} = \left( \sqrt{2} \gamma^{**} \sqrt{1 + \nu} \right) \left( E_f I_{\text{min}} / L_0^2 \right),
\]

where \( \nu \) is the Poisson ratio of the beam material. The critical force for Euler buckling for the same boundary conditions has a similar expression which differs by a constant:

![Figure 2.11](https://dummyimage.com/100x100/000/fff&text=Figure+2.11+%28a%29+Loading+of+a+beam+of+noncircular+cross-section+with+a+transverse+force,+and+%28b%29+lateral+buckling+during+bending+with+a+transverse+force+or+bending+moment.)
The critical moment for lateral buckling in pure bending may be arranged as 

\[ M_{cr} = \left( \sqrt{2\pi / \sqrt{1 + v}} \right) \left( E_f I_{min} / L_0 \right) \]. Therefore, the only moment of inertia relevant for the mechanics of such beams is that of the softer mode, \( I_{min} \). The deformation of the beam after instability takes place in the softer mode and hence \( I_{min} \) is also relevant for this situation.

In view of this observation, the mechanics of networks of slender fibers of noncircular cross-section is expected to be approximately similar to that of networks of fibers with circular section and with moment of inertia equal to the \( I_{min} \) value of the actual, noncircular fibers. This issue is discussed further in Section 6.1.1.3.7.

### 2.3.5 Crimped Fibers

Fibers are rarely straight in real networks. Therefore, accounting for the effect of fiber crimp (or tortuosity) in the analysis of fiber mechanical behavior is important.

Crimp is usually quantified using the parameter:

\[ c = \frac{L}{L_0} \], \hspace{1cm} (2.9)

where \( L \) is the length of the end-to-end vector of the fiber, while \( L_0 \) is the contour length. With a curvilinear coordinate, \( s \), taken along the contour of the fiber, \( L_0 = \int ds \). In all cases, \( c \leq 1 \).

To demonstrate the occurrence of crimp in network materials, Figure 2.12 shows the probability density function of collagen fiber crimp in the rabbit adventitia, the outermost layer of the carotid artery (Rezakhanli et al., 2012). The experimental distribution is well approximated by a beta distribution of coefficients \( \alpha = 4.47 \) and \( \beta = 1.76 \). The mean value of the tortuosity parameter in this case is \( c = 0.72 \).

It is currently thought that the presence of crimp in collagen fibers in arteries is physiologically necessary. Collagen and elastin form co-networks and provide the mechanical function of the tissue but play different roles. Elastin controls the linear elastic response of the tissue at small strains, while the collagen sub-network, which

![Figure 2.12](https://doi.org/10.1017/9781108779920.003)
has tortuous fibers, has limited contribution at small strains while the crimp is stretched out. At larger strains, the collagen network takes over and provides rapid stiffening, which limits tissue deformation and damage. Crimp values are different in different tissues, being smaller in connective tissue such as tendons.

Two cases are considered here in order to demonstrate the effect of crimp on the stiffness of nonstraight fibers, within the small deformation theory. The effect of crimp at constant fiber curvature is discussed first. To this end, a circular beam of radius $R$ is considered (Figure 2.13(a)) and the angle $\alpha$ describing the span of the beam is varied in the range $(0, \pi/2]$. In this problem, the crimp parameter results $c = \sin \alpha / \alpha$ and varies in the range $[2/\pi, 1)$. Second, we consider beams of the same crimp, but different curvature. This is discussed using the family of configurations shown in Figure 2.14(a). These fibers have the same crimp, $c = 2/\pi$, and increasing curvature. The axial stiffness of the fiber in Figure 2.13(a) is probed by applying a force $P_{ax}$ along the line connecting the two fiber ends and is computed using the Mohr–Maxwell method (Gere and Timoshenko, 2002). The effective stiffness, $k_{ax}^{\text{crv}}$, is compared with that of the straight beam of same end-to-end length, which is given by $k_{ax}^{\text{str}} = E_A f / 2R \sin \alpha$. Their ratio, $k_{ax}^{\text{crv}} / k_{ax}^{\text{str}}$, is shown in Figure 2.13(b) as a function of $\alpha$. $k_{ax}^{\text{crv}}$ is also a function of the ratio between the beam radius, $R$, and the cross-section diameter, $d$. Results for increasing $R/(d/2)$ are shown in Figure 2.13(b). The stiffness decreases rapidly with increasing $\alpha$ (decreasing $c$), and the effect is more pronounced as $R/(d/2)$ increases. Slender beams of small cross-section radius are very soft even at modest crimp.

Figure 2.13 (a) Configuration of a beam with crimp (curved beam) probed by forces acting along (axial) and perpendicular (bending) to the end-to-end vector. Variation of the ratio of the effective (b) axial and (c) bending stiffness of the curved and straight beams with angle $\alpha$. 
The bending stiffness of the beam in Figure 2.13(a) is probed by applying at the free end a force perpendicular to the end-to-end axis, \( P_{bd} \), and can be evaluated analytically using the same method. The stiffness is compared with that of the straight beam of same end-to-end length, which is given by

\[
k_{str}^{bd} = \frac{3E f l_f}{8R^3 \sin^3 \alpha}.
\]

The ratio \( k_{crv}^{bd} / k_{str}^{bd} \) is shown in Figure 2.13(c) and is insensitive to \( R = d/2 \). The bending stiffness reduction with increasing \( \alpha \) (decreasing \( c \)) is much less pronounced than in the case of the axial stiffness. The bending stiffness of this beam has the same value if the direction of the probing force, \( P_{bd} \), is reversed, despite the geometric asymmetry of the structure. Interestingly, it results that \( k_{crv}^{bd} / k_{str}^{bd} \) is approximately proportional to \( c = \sin \alpha / \alpha \) in this case.

The next example underlines the fact that crimp is not the only parameter of importance in this discussion; fiber stiffness changes rapidly when the curvature is varied. To demonstrate this effect, consider the family of beams shown in Figure 2.14(a). These beams are constructed by concatenating half-circles, and the number of half-circular units of each beam, \( n \), is varied. The total contour length is \( \pi R \), independent of \( n \). Since the end-to-end length is \( 2R \) in all cases, \( c = 2/\pi \) is \( n \)-independent. The beam curvature increases with \( n \) as \( n/R \). The ratio of the effective axial stiffness of the curved and straight beams becomes:

\[
\frac{k_{crv}^{ax}}{k_{str}^{ax}} = \frac{1}{\pi^4 + \pi (2\pi/\alpha)^3},
\]

(2.10)

and is shown in Figure 2.14(b) as a function of \( n \). With \( n \) varying from 1 to \( 4R/d \), the stiffness varies from that of the beam with the smallest curvature, \( 1/R \) (\( \alpha = \pi/2 \) in Figure 2.13(a)), to that of the straight beam. It results that the stiffness depends on both crimp and the actual shape of the beam.

The large deformation response of tortuous athermal fibers and the influence of their shape are demonstrated using data from Kabla and Mahadevan (2007). These authors consider fibers of shape described by a cosine function of given frequency and different amplitudes in the unloaded configuration and deform them in tension until
fully stretched. Figure 2.15 shows the force–crimp (equivalent to force–displacement) curves corresponding to fibers of initial tortuosity parameter $c = 0.46$, $0.85$, and $0.96$. The effective initial stiffness probed along the end-to-end axis increases with increasing $c$ of the undeformed configuration. The tangent stiffness decreases as the fiber is being pulled and then increases again as the fiber becomes almost straight and $c \to 1$.

If fibers are considered inextensible, the force–crimp curve has a vertical asymptote at a deformation corresponding to the fully stretched configuration. As this limit is approached, the force diverges as $P \sim 1/\sqrt{1 - c}$. It is instructive to compare this with similar results for the thermal filaments of freely rotating Langevin and semiflexible types discussed in Sections 2.4.1 and 2.4.4, respectively. In the present notation, the Langevin chain model predicts that the force diverges in the full extension limit as $P \sim 1/(1 - c)$ (Eq. (2.33)), while the semiflexible chain model predicts a faster divergence of the form $P \sim 1/(1 - c)^2$ (Eq. (2.51)). This comparison is aimed to just indicate the range of behaviors reproduced by these models that, in fact, represent different physics. The divergence of the force at $c = 1$ is eliminated if fibers are extensible.

These examples may appear simplistic in view of the fact that the shape of real fibers is always more complex than considered here. However, realistic fiber shapes may be described using a Fourier series as a superposition of trigonometric functions of increasing frequencies. At small deformations, their response is similar to that of a sinusoidal fiber of wavelength equal to the longest wavelength of the real fiber spectrum. This is due to the fact that fibers subjected to specified loads deform in the softest mode available – see the discussion in relation to Figure 2.6. The high frequency components of the fiber shape spectrum provide larger stiffness, as can be seen in the example of Figure 2.14. Therefore, the deformation begins by pulling out the low frequency waviness, while stretching the higher frequencies takes place at later stages and leads to gradual stiffening.

Closing the discussion of crimp, it is necessary to indicate the limitations of the measure of fiber tortuosity of Eq. (2.9). As discussed in more detail in Section 4.2.1, the crimp parameter is not an intensive quantity. It depends on the length scale of observation, $L_0$, if the largest wavelength of undulations is larger than or comparable...
with the contour length of the segment considered when evaluating the crimp parameter. If this wavelength is smaller than the probing length scale, crimp becomes a useful intensive geometric parameter, independent of the probing length. An alternative measure of tortuosity is the persistence length, $L_p$, which may be defined in both thermal and athermal cases, but is used extensively in thermal models (Section 2.4.2).

### 2.3.6 Inelastic Fiber Behavior

The mechanical behavior of athermal fibers probed in tension is generally elastic–plastic and may exhibit strain rate dependence. An important characteristic of the inelastic response is the yield stress. Most fibers exhibit yielding and the stress level at which plastic deformation begins depends on hydration, imposed deformation rate, thermal and deformation history of the fiber, etc. The strain rate sensitivity also depends on the state of the fiber and environmental conditions. Given this diversity of behaviors, providing a unified perspective similar to the description of the elastic response is not possible. Two examples are given next which provide an idea about the features of interest in the context of networks.

Figure 2.16(a) shows the stress–strain curve for a cellulose summerwood fiber, adapted from Seth and Page (1983). An initial elastic regime is followed by yielding at a stress of about 100 MPa and by plastic deformation with strain hardening. Residual strains result upon unloading and unloading–reloading cycles lead to limited hysteresis. The response changes greatly with the humidity level.

Figure 2.16(b) shows results from tensile uniaxial tests performed with a reconstituted collagen fiber of diameter ~200 nm (Liu et al., 2018). The fiber exhibits a slightly nonlinear response with no obvious yield point. A small residual strain results upon unloading and part of it recovers after the load is removed. Pronounced hysteresis is observed while performing loading–unloading cycles at constant maximum stretch. The fiber is viscoelastic, but a small plastic component cannot be excluded. The response is sensitive to hydration and temperature.
It is important to assess to what extent the inelastic fiber behavior is relevant for the mechanical behavior of networks. This issue is discussed quantitatively in Section 6.1.4. To address this question, it is necessary to consider the following points:

► Fibers of stochastic networks are loaded axially only at large strains and in networks of large fiber density which deform approximately affinely. In relatively sparse networks of thin filaments, such as most biological networks, nonwovens, felt, and other low-density network materials, fibers deform predominantly in their bending mode.

While plastic deformation may take place in bending, the probability of entering the plastic regime depends on the fiber diameter. A cantilever beam subjected to bending enters the plastic regime at a deflection which depends inversely on the fiber diameter. As the diameter is reduced below the micron range, very large deflections can be achieved while the fiber remains elastic. An impressive example of this type is provided by the glass fibers used in fiber optics which sustain very large bending deformations without failure or plastic deformation.

► In many network materials, the strain experienced by individual fibers is smaller than the strain imposed on the scale of the network. This is due to the nonaffine nature of deformation observed in most networks, and to the large geometric nonlinearity of the network behavior. The macroscale deformation is accommodated primarily by the reorganization of the network structure. This geometric effect, which allows the fibers to deform little even though the network-scale strains are large, is prevalent in low density networks.

Puxkandl et al. (2002) measured the strain experienced by fibers in a rat tendon sample by evaluating the D-spacing of the collagen fibrils. They compare the applied global strain with the fiber strain and conclude that the fiber strain is much smaller (below 30%) than the strain applied on the scale of the network. Considering that tendon is a strongly aligned collagen structure, the large difference between the local and global strains is particularly telling. In sparse networks with less pronounced preferential fiber alignment, this difference is expected to be even larger.

A similar conclusion was reached by Kabla and Mahadevan (2007) who performed experiments with felt made from randomly oriented polyester fibers of 30–50 μm diameter. Despite the global strains being close to 100%, it is reported that the fiber-scale strains remain limited, such that fibers, which have a yield strain in uniaxial tension of ~5%, remain elastic.

In the case of tortuous fibers, the gradual reduction of crimp during deformation allows for the accommodation of large network-scale strains with limited fiber-level deformation.

These considerations suggest that fiber inelasticity is expected to reflect in the network behavior only in dense and densely crosslinked networks and in networks of fibers with low critical stress for the onset of inelastic behavior. However, networks of thin fibers, of low density and/or with a low degree of cross-linking – which represent...
the vast majority of network materials of practical importance – are expected to be less sensitive to the inelasticity of the fiber constitutive behavior.\(^2\)

### 2.3.7 Fiber Strength and the Weibull Distribution

While the stiffness of a solid is an average property obtained by homogenization over the entire volume, the strength is governed by extreme value statistics. Strength is generally associated with the unstable propagation of a critical flaw, and hence depends on the probability to find such a flaw in a given body. This implies that the variability of the modulus values obtained in experiments with different samples is lower than the variability of the strength of the same sample set.

When testing fibers in uniaxial tension, material sub-domains (fiber segments) are connected in series and are loaded by the same stress. The failure of the weakest of these sub-domains entails the failure of the fiber.

Generally, failure of materials is represented with the Weibull distribution. Consider a fiber segment of length \(L\) and of strength described by the cumulative distribution:

\[
cp(\sigma) = 1 - \exp\left(-\left(\frac{\sigma}{\sigma_0}\right)^\beta\right),
\]

where \(cp(\sigma)\) represents the probability that failure takes place at a stress smaller or equal to \(\sigma\). Parameters \(\beta\) and \(\sigma_0\) are known as the Weibull modulus and the scale factor, respectively. Function \(cp(\sigma)\) increases from 0 to 1 as \(\sigma\) increases, with the fastest increase taking place in the vicinity of \(\sigma_0\) (if \(\beta > 1\)). The modulus, \(\beta\), controls how fast the probability increases and hence controls the variability of the strength values.

The probability density function results as the derivative \(d(cp)/d\sigma\):

\[
p(\sigma) = \frac{\beta}{\sigma_0} \left(\frac{\sigma}{\sigma_0}\right)^{\beta-1} \exp\left(-\left(\frac{\sigma}{\sigma_0}\right)^\beta\right),
\]

while the mean of the distribution is given by

\[
\sigma = \frac{\sigma_0}{\beta} \Gamma\left(\frac{1}{\beta}\right),
\]

and the variance is given by

\[
\text{var}(\sigma) = \sigma_0^2 \left[\Gamma\left(1 + \frac{2}{\beta}\right) - \Gamma^2\left(1 + \frac{1}{\beta}\right)\right].
\]

---

2 The fact that fibers remain in the elastic range does not mean that the behavior of the network is elastic. Inter-fiber friction, rupture of crosslinks, and the presence of an inelastic matrix may result in inelasticity on the network scale.
Figure 2.17(a) shows the variation of the normalized mean, $\overline{\sigma}/\sigma_0$, and variance, $\text{var}(\sigma)/\sigma_0^2$, with the Weibull modulus, for $\beta > 1$. The figure shows that the variance decreases fast as $\beta$ increases above $\approx 5$, and the mean approaches $\sigma_0$. Hence, the larger the Weibull modulus, the smaller the strength variability.

Figure 2.17(b) shows data for the strength of carbon fibers (Wu et al., 1991) with a 10 mm gauge length $L$, in a typical Weibull plot. The cumulative distribution of Eq. (2.11) is shown after taking the log twice on both sides, that is, one plots $\ln[-\ln(1-p(\sigma))]$ versus $\ln(\sigma)$. The slope of this plot is the Weibull modulus, $\beta$.

**Size effect:** Consider that experiments are performed with samples of length $L$ and a Weibull distribution of parameters $\beta$ and $\sigma_0$ represents the resulting data. It is of interest to inquire whether a different mean strength would be obtained if the experiments were performed with fibers of length $nL$ instead.

The probability of no failure at stresses below $\sigma$ for a fiber of length $L$ is

$$1 - cp(\sigma) = \exp\left(-\left(\frac{\sigma}{\sigma_0}\right)^\beta\right).$$  \hspace{1cm} (2.15)

The probability of no failure of all $n$ segments is the product of terms similar to Eq. (2.15). Therefore, the cumulative probability of failure below stress $\sigma$ of a fiber of length $nL$ is:

$$cp_n(\sigma) = 1 - \exp\left(-n\left(\frac{\sigma}{\sigma_0}\right)^\beta\right).$$  \hspace{1cm} (2.16)

The strength of the fiber of length $nL$ is characterized by a Weibull distribution of the same modulus, $\beta$, and of a scale factor equal to $\sigma_0n^{-1/\beta}$. The subscript $n$ indicates that the respective quantity refers to a fiber of length $nL$. 
This is an important result. It implies that the mean strength of fibers of length \( nL \) is:

\[
\bar{\sigma}_n = n^{-1/\beta} \sigma.
\]  

(2.17)

Therefore, the strength decreases continuously as the fiber length increases – a result also noted centuries ago by Leonardo da Vinci (see the collected works in da Vinci (1972)). Note that, since the modulus, \( \beta \), is rather large for most fibers of interest, \( 1/\beta \) is small and the size effect, although not negligible, may be rather weak.

The variance of the distribution of the strength of fibers of length \( nL \) may be computed with Eq. (2.14) and reads:

\[
\text{var}_n(\sigma) = n^{-2/\beta} \text{var}(\sigma).
\]  

(2.18)

The distribution becomes narrower as \( n \) increases. According to this model, the strength vanishes in the theoretical limit of \( n \rightarrow \infty \).

### 2.4 Thermal Filaments

Filaments whose mechanics are influenced by thermal fluctuations are called thermal. The average energy per degree of freedom provided by the thermal bath is \( k_B T/2 \), where \( k_B \) is Boltzmann’s constant. In ambient conditions, this is a small energy of the order of 0.025 eV, or \( 4 \times 10^{-21} \) J. Therefore, only very thin filaments that require small amounts of energy to deform can be classified as thermal. All molecular filaments in gels and polymeric materials, as well as most biomolecules, are thermal filaments. Even rather large molecules, such as the DNA and protein filaments (e.g., microtubules), are influenced by thermal fluctuations and belong to this class.

Filaments of very different bending stiffness may be classified as thermal. A polyethylene macromolecule is thin and flexible, while a polyisoprene molecule is also flexible, although less so than polyethylene. On the other hand, DNA is much stiffer in bending. For the same contour length, a flexible filament may assume many more configurations than a stiff thermal filament.

With this in mind, we discuss in this section the structure and mechanical behavior of three conceptual models of thermal filaments: (i) filaments made from rigid links which rotate freely relative to each other and may overlap as they explore the phase space of available conformations, (ii) similar filaments for which the links cannot overlap, and (iii) filaments composed of flexible links whose relative rotation is constrained to a narrow angular range. The first category is known as “freely rotating” or “ideal,” the second is known as “freely rotating with excluded volume,” while the third category is that of “semiflexible” filaments. Above the glass transition temperature, the effective behavior of such filaments is considered to be elastic and the elasticity is of entropic type.

A note on the terminology used is necessary. Since thermal filaments are studied by the polymer physics community, they are called “chains” (as in “polymeric chains”) in
the respective literature. In order to preserve consistency throughout this work, we prefer to refer to them with the more generic term of “filaments,” while distinguishing between fibers and filaments only based on the cross-section dimensions, as defined at the beginning of this chapter.

2.4.1 Freely Rotating Thermal Filaments

Consider a filament composed of $n$ rigid links of length $a$, which are pin-jointed and are free to rotate relative to each other (Figure 2.18(a)). Such filaments take random tortuous configurations under the action of thermal fluctuations. The excluded volume condition is not enforced and links of the filament can overlap other links. We are interested in determining the force required to deform such filaments. In this context, deformation refers to modifying the end-to-end length, $L$.

Since the links are rigid and no energetic interactions between links (nonbonded interactions) take place, the system has zero internal energy. However, due to the fact that the filament is free to sample all configurations available for given $L$, the entropy is not zero. The force in this model is purely entropic, that is, it results from the variation of the entropy during stretching. To see this, consider two extreme cases: one with the filament ends being co-located ($L = 0$), and the other with the filament being fully stretched ($L = na$). The number of configurations available to the chain in the first case is largest, while in the second case only one configuration is available. Therefore, the entropy decreases monotonically during stretching and this leads to an entropic force (Section 2.2).

2.4.1.1 Gaussian Model

We evaluate the probability of finding the filament in a configuration with given $L$. It is easier to begin the discussion by referring to the one-dimensional case and using an analogy with the one-dimensional random walk. Consider a walk of step length $a$, along axis $x$. The position of the walker after $n$ steps is given by $x = \sum_{i=1}^{n} q_i a$, where $q_i$ is $+1$ or $-1$, with equal probability, and the direction of the steps is uncorrelated.
along the walk. Then, the average position of the walker is \( \langle x \rangle = \sum_{i=1}^{n} \langle q_i \rangle a = 0 \). The mean square displacement, or the variance of the distribution of trajectory ends, is
\[
\langle x^2 \rangle = \sum_{i=1}^{n} q_i a \sum_{j=1}^{n} q_j a = a^2 \sum_{i=1}^{n} \sum_{j=1}^{n} \langle q_i q_j \rangle = na^2,
\]
where only terms with \( i = j \) survive in the double sum since the stochastic process \( q \) is not correlated.

The distribution of \( L \) can be found by simple arguments using the central limit theorem. This theorem indicates that the sum of \( n \) independent random variables is normal (Gaussian) distributed in the limit of large \( n \), with mean equal to the sum of the means of each variable in the sum, and variance equal to the sum of the respective variances.

For the one-dimensional random walk, the mean of individual steps is \( \langle x \rangle = 0 \), and the variance is \( \langle x^2 \rangle = a^2 \), and, hence, for the entire walk one obtains a mean of zero and variance of \( na^2 \). The corresponding distribution function for the one-dimensional walk (the probability to find the walker between \( x \) and \( x + dx \)), \( p_{1D} \), is:
\[
p_{1D}(x)dx = \frac{1}{\sqrt{2\pi na^2}} \exp \left( -\frac{x^2}{2na^2} \right) dx.
\]
This result may also be obtained by directly counting the number of possible paths leading from the origin to position \( x \), or by Fourier transform techniques, as done in some texts on polymer physics (Rubinstein and Colby, 2003) and in statistics texts (Weiner, 1983).

The result of Eq. (2.19) is restricted by the condition that \( n \) should be large. While this is generally true in practice, it is useful to note that, for small \( n \), the sum of independent variables follows an Irwin–Hull distribution. This distribution converges to the Gaussian rather rapidly; the Gaussian approximation is already reasonably accurate for \( n \geq 10 \).

Moving now to the three-dimensional space, we observe that the probability for a random walk of \( n \) steps, with the end-to-end vector being oriented in any direction in space, to end in the spherical layer bounded by \( L \) and \( L + dL \), is:
\[
p_{3D}(L) \cdot 4\pi L^2 dL = \int_{0}^{\pi} \int_{0}^{2\pi} p_{1Dp}(L \sin \theta \sin \varphi) p_{1Dp}(L \sin \theta \cos \varphi) p_{1Dp}(L \cos \theta) \sin \theta L^2 d\theta d\varphi dL,
\]
where \( \theta, \varphi \) are the Euler angles of the end-to-end vector. The probability density \( p_{1Dp} \) corresponding to the projection of the path along some axis which does not coincide with the end-to-end vector is, by the arguments based on the central limit theorem discussed in relation to Eq. (2.19), a Gaussian of mean zero and variance \( na^2/3 \). Replacing Eq. (2.19) in Eq. (2.20) leads to the probability density function for the end-to-end length of the walk as:
\[
p_{3D}(L) = \left( \frac{3}{2\pi na^2} \right)^{3/2} \exp \left( -\frac{3L^2}{2na^2} \right)
\]
(2.21)
Equation (2.21) represents a Gaussian distribution for the end-to-end vector length. The corresponding unit vector is uniformly distributed over the sphere of unit radius. Obviously, the mean of the distribution is zero, while the variance of \( L = |\mathbf{L}| \) is \( na^2 \). We further use the notation \( L^* = a\sqrt{n} \) for the representative measure of the end-to-end distance of the filament.

We are now in the position to evaluate the entropic force required to stretch the filament. We consider first situations in which small variations of \( L \) are applied to a filament with \( L^* = a\sqrt{n} \ll L_0 = na \). For large \( n \), such configurations represent states in which the end-to-end distance of the filament is much smaller than the fully stretched (contour) length, that is, situations in which the representation of the filament as a random walk is appropriate. Note that the distribution of Eq. (2.21) is only valid for an undirected random walk. If the filament is stretched such that \( L \) is smaller than, but comparable with the contour length, \( L_0 \), one may use a directed random walk model, which leads to statistics different from Eq. (2.21).

With this limitation in mind, we consider that \( L \) is the control parameter and evaluate the variation of the filament entropy associated with a small variation of \( L \). The entropy \( \Sigma \) is computed using:

\[
\Sigma = k_B \ln \Omega(L),
\]

where \( \Omega(L) \) is the total number of configurations available to a filament of \( n \) links with end-to-end length \( L \). This is related to the probability of Eq. (2.21) as:

\[
p_{3D}(L) = \frac{\Omega(L)}{\int \Omega(L)dL},
\]

and, therefore,

\[
\Sigma = k_B \ln p_{3D}(L) + k_B \ln \int \Omega(L)dL.
\]

The second term in Eq. (2.24) is only a function of \( n \) and remains constant if \( L \) changes. With Eq. (2.21), Eq. (2.24) becomes:

\[
\Sigma = -\frac{3k_B L^2}{2na^2} + g(n),
\]

where terms independent of \( L \) are represented by \( g(n) \).

The ensemble considered here is similar to the canonical ensemble in which the number of particles, the kinematic parameters, and the temperature are controlled. The only kinematic parameter in this problem is \( L \). In these conditions, the appropriate potential function is the Helmholtz free energy, \( \Psi \), seen in Eq. (2.1).

The force required to change the end-to-end length of the filament, \( \mathbf{P} \), is obtained using Eq. (2.3). The energy of the filament is zero and hence only the entropic term remains, which leads to:

\[
\mathbf{P} = -T \frac{\partial \Sigma}{\partial L}.
\]
Equation (2.26) shows that the force is aligned with $\mathbf{L}$. Using Eq. (2.25), the magnitude of the force is

$$P = k_BT \frac{3L}{n\alpha^2} \quad (2.27)$$

This expression exhibits two important features. The force is proportional to the temperature. This is the signature of its entropic nature. To see the difference relative to a fiber with energetic stress, consider a metallic rod held in a stretched configuration and further subjected to an increase of temperature. The temperature has no effect on the stress-production mechanism. However, thermal expansion causes the rod to dilate and hence the axial tensile force decreases with increasing temperature. Equation (2.27) predicts the opposite behavior: the force in the filament increases as the temperature increases. This type of behavior was observed in rubber at the beginning of the twentieth century, which opened the way to the development of the now classical theory of rubber elasticity which assumes that stress in this network material is purely entropic.

The second important feature of Eq. (2.27) is that the force is proportional to the end-to-end distance $L$. Hence, the filament behaves as if it were a spring of axial stiffness $3k_BT/n\alpha^2$ with a force that vanishes only when the two ends of the filament are co-located ($L = 0$). The filament with any nonzero $L$ is subjected to a tensile force. The natural question that arises is why polymeric chains do not always have a zero end-to-end distance. Another force must be present to provide the necessary balance and ensure a distribution of end-to-end vector lengths. It is generally assumed that this reaction force is provided in a dense material by the excluded volume interactions (repulsion between monomers forming the filaments).

The model described in this section is the Gaussian model of the thermal filament. It is limited in scope to small stretches. To develop a more suitable representation, it is necessary to account for large deformations, including situations in which $L$ becomes comparable with the contour length of the filament, $L_0$.

### 2.4.1.2 Langevin Model

Consider now the problem of chain extension under force control, with $P$ being the force stretching the filament. The current ensemble is similar to the isothermal–isobaric ensemble in which the number of particles, the stress (or force), and the temperature are the control parameters. The relevant thermodynamic potential in this case is the Gibbs free energy.

In statistical mechanics, the Gibbs free energy, $\widehat{G}$, is related to the partition function of the isothermal-isobaric ensemble, $Z_f$, as:

$$\widehat{G} = -k_BT \ln Z_f. \quad (2.28)$$

For a system with zero internal energy, $U = 0$, on which external forces do work, the partition function $Z_f$ is expressed as an integral of the Boltzmann factor computed based on the enthalpy, performed over all possible conformations compatible with the given force:
Here it is made explicit that the variable $L$ conjugated with the applied force is a function of the spatial orientation of the $n$ links described by the Euler angles, $\theta_i$ and $\phi_i$, $i = 1 \ldots n$, measured relative to the direction of the force $P$. The $2n$ Euler angles define the phase space of the problem. The product $P \cdot L$ is the work performed by the force on the system (hence the sign convention). The end-to-end distance can be written in terms of $\theta_i$ as $L = a \sum_{i=1}^{n} \cos \theta_i$ and the work can be written $P \cdot L = Pa \sum_{i=1}^{n} \cos \theta_i$. Then, the integral in Eq. (2.29) can be evaluated leading to:

$$Z_f = \prod_{i=1}^{n} \exp \left( \frac{Pa \cos \theta_i}{k_B T} \right) \sin \theta_i \sin \phi_i \int \exp \left( \frac{Pa \cos \theta}{k_B T} \right) \sin \theta d\theta d\phi = \left[ 4\pi \sinh \frac{Pa}{k_B T} \right]^{n}.$$  (2.30)

The elimination of the product in the first equality is possible because all $i$ links sample the same sub-space defined by $\theta_i$ and $\phi_i$. Then, the product can be factored out and the integrals remaining under the product are identical.

Using Eqs. (2.28) and (2.30), the Gibbs free energy can be computed as:

$$\tilde{G} = -nk_B T \left[ \ln \left( \sinh \frac{Pa}{k_B T} \right) - \ln \left( \frac{Pa}{k_B T} \right) + \ln 4\pi \right].$$  (2.31)

$L$ may be computed from the thermodynamic potential as:

$$L = -\frac{\partial \tilde{G}}{\partial P} = na \left[ \coth \left( \frac{Pa}{k_B T} \right) - \frac{k_B T}{Pa} \right] = naL \left( \frac{Pa}{k_B T} \right) = L_0 \tilde{L} \left( \frac{Pa}{k_B T} \right),$$  (2.32)

where function $\tilde{L}(x) = \coth(x) - 1/x$ is known as the Langevin function. The normalized force, $Pa/k_BT$, is expressed in terms of the inverse Langevin function as $Pa/k_BT = L^{-1}(L/L_0)$. The inverse Langevin function can be approximated with Padé’s formula as $L^{-1}(x) \approx x(3 - x^2)/(1 - x^2)$, which provides values within 3% of the actual function for $L/L_0 \leq 0.8$ (Cohen, 1991).

An alternative derivation can be performed in the canonical ensemble, with the control variable being the filament end-to-end distance, as described in, for example, Weiner (1982).

Equation (2.32) describes the constitutive behavior of the thermal filament with no constraints on the magnitude of the deformation. The relation between the force and the mean end-to-end length resulting from the inversion of Eq. (2.32) is shown in Figure 2.19 along with the prediction of the Gaussian filament model, Eq. (2.27). The Langevin model predicts stiffening at large elongations, while the Gaussian model predicts constant linear stiffness of magnitude $3k_BT/na^2$ at all stretches.
In both models, the normalized force $Pa/k_BT$ is related to the ratio $L/L_0$ through a universal relation independent of $n$, which fully defines the stiffening behavior of the filament in tension.

In the large force limit, the Langevin function can be approximated as

$$L(x) \approx 1 - 1/x.$$  

The normalized force diverges when the end-to-end distance $L$ approaches the filament contour length $L_0$ as:

$$\frac{Pa}{k_BT} \approx \frac{L_0}{L_0 - L} = \frac{1}{1 - c},$$  

an asymptotic behavior which is also independent of $n$.

The fact that the response stiffens rapidly at large stretches indicates that the variation of the entropy, that is, the variation of the total number of conformations available to the filament corresponding to a given increment of the stretch, is more rapid when the chain is almost fully stretched. Furthermore, in the Gaussian filament case, an increment of stretch reduces the entropy associated with the long wavelength modes faster. This situation is similar to that of athermal fibers in which, likewise, stiffness is primarily controlled by the long wavelength undulations (Section 2.3.5).

It is important to emphasize that the filament only responds to forces aligned with its end-to-end vector. Transverse forces perform no work since the entropy does not vary when the two ends of the filament rotate relative to each other, while maintaining constant their relative distance. It results that thermal filaments can be modeled with linear (Gaussian) or nonlinear (Langevin) axial springs. The choice of the filament model has significant consequences for the mechanics of networks made from thermal filaments.

### 2.4.2 Persistence Length

In Sections 2.4.1.1 and 2.4.1.2 it was assumed that the filament is composed from links of specified length, $a$, which are free to rotate relative to each other.
(Figure 2.18(a)). It is of interest to analyze cases in which filaments are less flexible. To this end, we consider a slightly modified model in which the angle made by a link relative to the previous link is selected from a uniform distribution in the range \((-\alpha, \alpha)\) (Figure 2.18(b)). If \(\alpha\) is relatively small, the filament is less curvy on scales comparable with \(a\), but it resembles the freely rotating model on scales much larger than \(a\). Therefore, a length scale exists which separates these two types of behavior. To define it, we evaluate the rate of decay of the link orientation correlation function along the contour of the filament. In the two-dimensional case, the directional correlation is computed as:

\[
C(m) = \langle t_i \cdot t_{i+m} \rangle_i = \left\langle \cos \left( \sum_{j=1}^{m} \Delta \theta_{j,j+1} \right) \right\rangle,
\]

where \(t_i\) is the filament tangent unit vector at the location of link \(i\) and \(t_{i+m}\) is the tangent unit vector \(m\) links away. The average is performed over all realizations and/or along the filament, for various \(i\) values. \(\Delta \theta_{j,j+1}\) is the angle between link \(j\) and the subsequent link \(j+1\). The random independent variables \(\Delta \theta_{j,j+1}\) are distributed with zero mean and variance \(\alpha^2/3\).

\[
\sum_{j=1}^{m} \Delta \theta_{j,j+1}\]

follows an Irwin–Hall distribution which converges to the Gaussian distribution for sufficiently large \(m\) (approximately \(m \geq 10\)). The resulting Gaussian has zero mean and variance \(ma^2/3\). Hence, the average in Eq. (2.34) can be computed and the correlation function results:

\[
C(m) = \exp \left( -\frac{ma}{6a^2/\alpha^2} \right).
\]

The correlation function of the tangent vector decays exponentially with the number of steps (each having length \(a\)) along the filament. The emerging length scale is \(6a/\alpha^2\), which is the correlation length of the filament tangent vector orientation, also known as the persistence length, \(L_p\):

\[
\frac{L_p}{a} \approx \frac{6}{\alpha^2},
\]

where the approximate sign is introduced to account for the assumption of large \(m\) made in the derivation.

For contour lengths smaller than \(L_p\), the filament appears approximately straight, while for much larger contour lengths, it resembles the freely rotating filament discussed in Section 2.4.1. The normalization of all lengths by \(L_p\) (more exactly by \(2L_p\), which is known in polymer physics as the Kuhn length), renders this type of filament equivalent to the freely rotating one.

The derivation is more complicated in three dimensions due to the additional random rotation of link \(j+1\) relative to link \(j\). It is nevertheless possible to show that the correlation function decays exponentially:

\[
C(m) \sim \exp \left( -\frac{ma}{L_p(a)} \right).
\]
The analysis in this section is purely geometric and is independent of the nature of the filament. It applies equally to thermal and athermal cases. In the thermal case of semiflexible filaments, the persistence length can be computed based on the bending rigidity of the filament (Eq. (2.49)). In the athermal case, in which filaments are continuous (not made from links, as in Figure 2.18), the average of Eq. (2.34) can be computed identically based on the filament tangent unit vectors.

2.4.3 Role of the Excluded Volume

We now take one more step toward eliminating the approximations inherent in the freely rotating model of thermal filaments, which assumes that links are phantom and may freely overlap and cross each other. The self-avoiding random walk model imposes the excluded volume constraint which prevents chain segments from overlapping and crossing. The statistics of the filament end-to-end distance is modified in this representation relative to the freely rotating model, but the entropic nature of stress is preserved.

The self-avoiding random walk was studied by a large number of researchers starting from the middle of the twentieth century. Nevertheless, the number of analytic results available is relatively small and generally applicable only for large \( n \).

Numerical evidence and scaling arguments suggest that the representative measure of the end-to-end distance, \( L^* \), results in this case:

\[
L^* = \sqrt{\langle L^2 \rangle} \sim an^\gamma, \tag{2.38}
\]

where \( \gamma \) is an exponent that depends on the dimensionality of the embedding space. Fisher (1969) used ideas developed by Flory (1949) to provide an approximation for the exponent:

\[
\gamma = \begin{cases} 
\frac{3}{4} & 2D \\
\frac{3}{5} & 3D
\end{cases}. \tag{2.39}
\]

Comparing with the freely rotating model for which \( \gamma = 1/2 \), the larger \( \gamma \) value indicates that the size of the filament increases significantly when the no overlap condition is enforced. The filament remains a fractal object, but the fractal dimension (which is equal to \( 1/\gamma \)) increases from 2 in the freely rotating model, to 5/3 (in 3D) in the self-avoiding representation.

The simplest explanation for the scaling of Eq. (2.38) is given by the model due to Flory (1949). This theory provides a physical justification for the swelling of the self-avoiding filament. Consider a filament made from \( n \) links that occupies the sphere of radius equal to the end-to-end length, and of volume proportional to \( \sim L^*^3 \). If the volume of one link is \( v \), and all links occupy a volume \( nv \), the probability of overlap is \( p_{ov} = nv/L^*^3 \). An energy penalty for overlaps is introduced, of magnitude \( \varepsilon \) per overlap. Therefore, the energy associated with packing is \( \sum_{i=1}^n \varepsilon p_{ov} \sim \varepsilon n^2 v/L^*^3 \). At the same time, the entropic contribution to the free energy is the entropy of the filament of end-to-end distance \( L^* \). Flory uses the result for the Gaussian

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filament, Eq. (2.25), to approximate the entropy. The resulting free energy contribution is proportional to \(k_B T L^* n^2/na^2\). The total free energy becomes \(q_1 e n^2/V/L^* + q_2 k_B T L^* n^2/na^2\), where \(q_1\) and \(q_2\) account for constants not made explicit in the expressions of the two components of the free energy. The equilibrium configuration is obtained by minimizing the free energy with respect to \(L^*\). Taking the derivative of the free energy expression with respect to \(L^*\) and setting it to zero leads to the scaling relation \(L^*/C_24 n^3 = 5\); hence the exponent \(\gamma\) of Eq. (2.39) results.

Beginning with Fisher (1966), Chay (1970), des Cloizeaux (1974), and de Gennes (1979), many authors sought to establish the probability density function of the end-to-end distance of the self-avoiding random walk. It is considered that the probability density for large \(n\) values is of the form:

\[
p_{3D}^{sa}(L) \sim \left(\frac{L}{L^*}\right)^\beta \exp \left( -\frac{3}{2} \left(\frac{L}{L^*}\right)^\delta \right),
\]

(2.40)

Fisher (1966) suggests that the exponent \(\delta\) is related to exponent \(\gamma\) in Eq. (2.38) as \(\delta = 1/(1 - \gamma)\).

\(p_{3D}^{sa}\) decreases to zero when \(L \to 0\), which is expected considering that the energy penalty associated with packing diverges in this limit. \(p_{3D}^{sa}\) has a maximum for intermediate values of \(L\) and decreases to zero at large \(L\). In this limit, packing is less important and the Gaussian-like statistic prevails, albeit with different exponents reflecting the self-avoiding walk statistics.

With Eq. (2.40), one may follow the procedure described for the Gaussian filament (Eqs. (2.25)–(2.27)) to derive the force required to stretch the filament:

\[
\frac{P_a}{k_B T} = \frac{3}{2} \frac{1}{1 - \gamma} \left(\frac{L}{L^*}\right)^{\gamma} \frac{a}{L^*} - \frac{\beta a}{L^*}.
\]

(2.41)

In the freely rotating filament case, \(\gamma = 1/2\) and the excluded volume effect disappears, which requires \(\beta = 0\), and, with \(L^* \sim an^2\), Eq. (2.41) reduces to Eq. (2.27). The first term represents the entropic effect and is similar to the Gaussian filament case, while the second term is a consequence of packing and has the effect of swelling the filament. The first term dominates at large \(L\) and the second term contribution is important at small \(L\). For \(\gamma = 3/5\), Eq. (2.39), Eq. (2.41) predicts a nonlinear increase of the force as \(P_a/k_B T \sim (L/L_0)^{3/2}\); note that \(L_0 = na\).

It should be observed that the nonlinearity of the present model originates from the statistic of the walk and is different from the nonlinearity of the Langevin filament, which is associated with the nonquadratic variation of the entropy with the filament stretch at large filament extensions.

### 2.4.4 Semiflexible Filaments

Semiflexible filaments are thermal filaments for which the energetic contribution of the bending modes cannot be neglected. Imagine an initially straight filament which is allowed
to fluctuate under the action of thermal excitation. The primary deformation mode is bending, which, for slender filaments of common interest, is much softer than the axial mode. Hence, the filament performs random bending oscillations and these fluctuations influence the response to axial loading. Stretching leads to a reduction of the number of configurations available to the filament. Most biopolymers are semiflexible; examples include DNA, microtubules, actin, and fibrin. Single wall carbon nanotubes may also be regarded as semiflexible filaments. In all these cases, the persistence length is large and often comparable with, or even larger than, the end-to-end length of the filament. The tortuosity (crimp) of semiflexible filaments is reduced relative to the fully flexible case. This strongly contrasts with the case of some synthetic polymers and rubber, in which the persistence length is small and the tortuosity is pronounced. Therefore, it is expected that the mechanics of semiflexible filaments is different from that of flexible filaments.

The classical model for semiflexible filaments is the worm-like chain (WLC) model due to Kratky and Porod (1949). Following the statistical mechanics solutions provided in Marko and Siggia (1995) and Odijk (1995), many researchers contributed to the development of this model (e.g., Moroz and Nelson, 1998; Boucilit et al., 1999; Dobrynin et al., 2010). Here we present the conceptual outline of the model, without going into the details of the derivation, for which the reader is referred to the cited literature.

Consider a filament of length $L_0$, which is straight in the absence of thermal fluctuations, fixed at one end and loaded by a force $P$ at the free end (inset to Figure 2.20(b)). The tensile force is aligned with the filament axis and produces no bending if the filament is in the straight, unperturbed configuration. The filament becomes undulated due to thermal excitations and its end-to-end length, $L$, decreases as the temperature increases. Increasing the axial force leads to the reduction of the fluctuation amplitude and to an increase of $L$. The objective here is to evaluate the relation between $L$ and the applied force.

![Figure 2.20](https://doi.org/10.1017/9781108779920.003) Published online by Cambridge University Press

Figure 2.20 (a) Normalized force $PL_0^2/E_f I_f$ versus the chain crimp parameter $L/L_0$, as predicted by the WLC model of Eq. (2.48). At zero force $L/L_0 < 1$ due to thermal fluctuations and $L$ decreases with increasing temperature. (b) One of the curves in (a) shown in semi-log plot with a larger range of forces to demonstrate the divergence at $L \rightarrow L_0$. The inset shows a schematic of the WLC model and the notation used.
The potential energy of the filament includes an energetic component associated with bending, and a work term, and can be obtained from Eq. (2.5):

\[
PE = \frac{1}{2} \int_{0}^{L_0} E_f I_f \left( \frac{d\theta(s)}{ds} \right)^2 ds - P \cdot u(L_0). \tag{2.42}
\]

The axial deformation mode is neglected here (but considered in the derivation in Odijk (1995)), \(d\theta(s)/ds\) is the curvature of the filament, and \(u(L)\) is the displacement at the free end of the filament, at \(x = L\) (or \(s = L_0\)). Note that if large rotations and deformations are allowed, all bending, axial, and torsional modes are engaged and the mechanics of the filament becomes more complex. The statistical mechanics of this case is discussed in Moroz and Nelson (1998). For simplicity, here we consider \(P\) and \(u\) to be aligned in the \(x\)-direction and hence \(P \cdot u(L_0) = P \left( \int_{0}^{L_0} \cos \theta ds - 0L \right)\), where \(P = |P|\) and \(0L\) is the end-to-end length when \(P = 0\) and thermal fluctuations are present (\(0L < L_0\)). Assuming further that the departure from the straight configuration is small, \(\cos \theta \approx 1 - \theta^2/2\), the potential energy reads:

\[
PE = \frac{1}{2} \int_{0}^{L_0} E_f I_f \left( \frac{d\theta(s)}{ds} \right)^2 ds + \frac{1}{2} P \int_{0}^{L_0} \theta^2 ds - P(0L - 0L). \tag{2.43}
\]

The filament shape is defined by \(\theta(s)\). This function is expanded in a Fourier series:

\[
\theta(s) = \sum_{n=1}^{\infty} \alpha_n \sin \frac{\pi ns}{L_0} + \beta_n \cos \frac{\pi ns}{L_0}. \tag{2.44}
\]

The filament is considered pinned at both ends, which implies that no moments are applied at either end and the curvature, \(d\theta/ds\), vanishes at the filament ends. This requires \(\alpha_n = 0\), and only the second term in Eq. (2.44) remains. With this, the potential energy can be written as:

\[
PE = \sum_{n=1}^{\infty} \beta_n^2 \left[ E_f I_f \frac{\pi^2 n^2}{4L_0} + \frac{PL_0}{4} \right] - P(0L - 0L). \tag{2.45}
\]

Thus far the mechanics of the filament is described in energetic terms. In the next step, an average of Eq. (2.45) is performed and the equipartition theorem is used requiring that each mode of the energetic component carries, on average, an energy equal to \(k_BT/2\). Then, \(\langle \beta_n^2 \rangle\) can be computed as:

\[
\langle \beta_n^2 \rangle = \frac{2k_BT L_0}{E_f I_f \pi^2 n^2 + PL_0^2}. \tag{2.46}
\]

In 3D, the filament oscillation modes in the two directions orthogonal to the filament axis are statistically independent and hence two modes correspond to each \(n\). Therefore, the energy corresponding to each \(n\) is \(k_BT\).
The mean end-to-end length of the filament can be computed as:

\[ \langle L \rangle = \int_0^{L_0} \langle \cos \theta \rangle ds \approx L_0 - \frac{1}{2} \int_0^{L_0} \langle \theta^2 \rangle ds, \]  

(2.47)

and with Eqs. (2.44) and (2.46), it results that

\[ 1 - \frac{\langle L \rangle}{L_0} = \frac{1}{2L_0} \int_0^{L_0} \langle \theta^2 \rangle ds = \frac{1}{4} \sum_{n=1}^{\infty} \langle \beta_n^2 \rangle = \frac{1}{2L_p} \frac{1}{\sqrt{\tilde{P}}} \left( \coth \sqrt{\tilde{P}} - \frac{1}{\sqrt{\tilde{P}}} \right), \]  

(2.48)

where \( \tilde{P} = PL_0^2/E_f I_f \) is a non-dimensional version of the force \( P \). The last expression in Eq. (2.48) is evaluated with Eq. (2.46).

The quantity

\[ L_p = \frac{E_f I_f}{k_BT} \]  

(2.49)

is the persistence length of a semiflexible filament in 3D. In two dimensions (the derivation presented here is performed in 2D), \( L_p = 2E_f I_f/k_BT \).

Expanding in series the right side of Eq. (2.48) in the vicinity of \( \tilde{P} = 0 \) and retaining only the first term in \( \tilde{P} \) leads to

\[ 1 - \frac{\langle L \rangle}{L_0} = \frac{1}{2L_0} \int_0^{L_0} \langle \theta^2 \rangle ds = \frac{1}{4} \sum_{n=1}^{\infty} \langle \beta_n^2 \rangle = \frac{1}{2L_p} \frac{1}{\sqrt{\tilde{P}}} \left( \coth \sqrt{\tilde{P}} - \frac{1}{\sqrt{\tilde{P}}} \right), \]  

(2.48)

where \( \tilde{P} = PL_0^2/E_f I_f \) is a non-dimensional version of the force \( P \). The last expression in Eq. (2.48) is evaluated with Eq. (2.46).

The quantity

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is the persistence length of a semiflexible filament in 3D. In two dimensions (the derivation presented here is performed in 2D), \( L_p = 2E_f I_f/k_BT \).

Equation (2.46) indicates that the equipartition theorem establishes a power spectrum of the filament shape which decays as the inverse of the square of the frequency (with and without an applied force). The Wiener–Khinchin theorem relates the autocorrelation function to the power spectrum (the power spectrum is the Fourier transform of the autocorrelation function) and mandates that, for a spectrum of this type, the autocorrelation function is of the exponential type. Hence, the exponentially decaying correlation function of Eq. (2.37) originates from the modal distribution of energies of the flexible filament subjected to thermal fluctuations. The persistence length of Eq. (2.37) results from this analysis and is given by Eq. (2.49). An alternate derivation of the persistence length is provided in Howard (2001).

Eq. (2.48) should be compared with the equivalent equation describing the freely rotating Langevin chain, Eq. (2.32), which can be rearranged in a format similar to that of Eq. (2.48) and reads:

\[ 1 - \frac{\langle L \rangle}{L_0} = 1 - \coth \tilde{P} + \frac{1}{\tilde{P}}, \]  

(2.50)

where \( \tilde{P} = Pa/k_BT \). The limit of the right side of Eq. (2.50) for \( P \to 0 \) is 1, which indicates that in the absence of applied force, \( \langle L \rangle = 0 \), as expected for the freely rotating model.

It is of interest to evaluate the behavior of the semiflexible model in the two limits of small and large \( P \). The assumption of small departures from the straight
configuration renders the model inaccurate in the limit of small forces, when slack may be significant. Nevertheless, it can be inferred from Eq. (2.48) that for \( P \to 0 \) the average end-to-end length of the filament, \( \langle 0L \rangle \), is given in the first order by \( \langle 0L \rangle / L_0 \approx 1 - L_0 / (6\ell_p) \).

In the limit of large forces, when \( \langle L \rangle \) approaches \( L_0 \), the force diverges as:

\[
P \sim \frac{1}{(L_0 - \langle L \rangle)^2} \sim \frac{1}{(1 - c)^2}.
\]

(2.51)

This is in contrast with the behavior of the freely rotating Langevin chain for which the force diverges at large extensions as \( P \sim 1/(1 - c) \) (Eq. (2.33)). The force enters the regime described by Eq. (2.51) for \( P > 5 \) or \( 1 - \langle 0L \rangle / L_0 < 0.128 \) \( L_0 / \ell_p \), which is quite close to the unloaded state characterized by \( 1 - \langle 0L \rangle / L_0 \approx L_0 / 6\ell_p = 0.166 \) \( L_0 / \ell_p \). Therefore, the model essentially has no linear elastic regime.

The worm-like chain response of Eq. (2.48) is shown in Figure 2.20(a) for several values of \( \ell_p / L_0 \).

In the derivation of Eq. (2.48), the equipartition theorem is applied to the potential energy given by Eq. (2.45), leading to the set of coefficients \( \beta_n^2 \) of Eq. (2.46). This implies that equipartition applies at all times as the filament deforms under load. It is of some interest to compare this situation with an equivalent athermal case in which a static, nonthermally fluctuating filament of initial, stress-free state defined based on the frequency spectrum of the thermal filament is loaded axially (van Dillen et al., 2008). This athermal filament model leads to a constitutive behavior similar to that of Eq. (2.48), except that the second term in the parentheses, \( 1 / \sqrt{P} \), is replaced by \( \sqrt{P} / \sinh^2 \sqrt{P} \) and the \( 1/2 \) coefficient in front of the right hand side becomes \( 1/4 \). The athermal filament of shape defined by the same statistics as the WLC filament is softer than its thermal counterpart. It should be noted though that a generic athermal filament is not expected to have a shape defined by a spectrum similar to that of the WLC. Spectra defining the shape of filaments extracted from a felt and their effective force–stretch response are presented in Kabla and Mahadevan (2007).

The behavior of many semiflexible filaments has been measured in recent years by direct probing using optical tweezers. In this type of experiment, two beads are connected to the two ends of the filament and are then trapped in the focal region of two highly focused laser beams. The beads are attracted or repelled by the beams function of the difference of the refractive index of the bead and the surrounding medium. This allows manipulating the beads by moving the laser beams which makes possible applying pN level forces on the probed filament. The experiment allows evaluating of the force–extension curve of the filament.

Typically, the WLC model is fitted to the measured force–extension curve, which provides an estimate of the filament persistence length. An example is shown in Figure 2.21, where experimental data from stretching a DNA molecule of \( L_0 = 15.6 \) \( \mu \text{m} \) in 10 mM PB buffer is presented (Strick et al., 1996). The line represents the fitted WLC model. The persistence length of the filament results as \( \ell_p = 51.3 \pm 2 \) nm.
A useful approximation to the force–extension relation predicted by the WLC model of Eq. (2.48) was proposed by Bustamante et al. (1994) and has the explicit form:

\[
P \approx \left( \frac{L_0}{L_p} \right)^2 \left[ \frac{1}{4} \left( \frac{1}{\sqrt{y^2}} - 1 \right) + 1 - y \right],
\]

(2.52)

where \( y = 1 - x/L_0 \) and \( x \) is the extension given by \( x = \langle L \rangle - \left( L_0 - \frac{L_0^2}{6L_p} \right) \). Another approximation is proposed in Bouchiat et al. (1999). The quality of these approximations depends strongly on \( L_0/L_p \). For \( L_0/L_p = 0.5 \), Eq. (2.52) is within 10% of Eq. (2.48) only when \( \langle L \rangle/L_0 > 0.97 \), that is, for almost straight filaments. For a more flexible filament, with \( L_0/L_p = 50 \), requiring 10% accuracy restricts the range of applicability of Eq. (2.52) to \( \langle L \rangle/L_0 > 0.87 \).

Comparing the WLC model with other models of thermal filaments, it is useful to recall computer simulation results for filaments with bending stiffness. It has been observed (Livadaru et al., 2003; Rosa et al., 2003) that such chains exhibit two regimes of behavior: the response can be represented by the WLC model at relatively small forces, with the force scaling as \( P \sim (L_0 - \langle L \rangle)^{-2} \sim 1/(1 - c)^2 \) (Eq. (2.51)), while at forces larger than some threshold, the response is similar to that of the freely rotating chain model, with the force scaling as \( P \sim (L_0 - \langle L \rangle)^{-1} \sim 1/(1 - c) \) (Eq. (2.33)). The crossover force increases with increasing the bending rigidity of the filament, \( E_f I_f \). An analytic derivation of a model capturing this behavior is presented in Dobrynin et al. (2010) along with results from experiments on isolated synthetic and biological molecules and computer simulation data supporting the proposed concept.

2.5 Mechanics of Fiber Bundles

In most natural and some man-made network materials, the network is composed from fiber bundles, as opposed to individual fibers. Collagen fibers of the extracellular...
matrix and connective tissue are bundles of tropocollagen fibrils. Buckypaper is a stochastic network of bundled carbon nanotubes stabilized by strong cohesive interactions between nanotubes. Virtually all composite materials with continuous fibers are made from fiber bundles (fiber tows), which are woven to produce prepregs. The vast majority of the threads used in the textile industry are bundles (yarns) of discontinuous natural fibers. Therefore, it becomes apparent that in the discussion of the mechanical behavior of network materials, the behavior of fiber bundles is at least as relevant as that of individual fibers.

Figure 2.22 shows schematics of fiber bundles of continuous fibers. An idealized bundle of fibers arranged parallel to each other is shown in Figure 2.22(a). Figure 2.22(b) shows schematically that fibers may exhibit waviness and exchange their relative position within the bundle. Fiber waviness leads to packing defects that increase the total volume of the bundle. Fiber tows used in composites usually exhibit this type of bundle structure. The packing and ordering of fibrils within collagen fibers is poorly described in the current literature. However, it is expected that configurations of the type shown in Figure 2.22(b) are also prevalent in collagen.

Virtually all textile yarns are twisted (Figure 2.22(c)). Twisting increases the total length of fiber per unit length of the bundle, but greatly improves the mechanical properties of the yarn. Fibers in a twisted yarn have approximately helical trajectories. A force acting along the bundle axis tends to reduce the radius of the helix and hence produces a compressive radial stress. This enables frictional interactions between fibers, which assists inter-fiber load transfer. This mechanism provides strength to yarns made from discontinuous fibers which, in the absence of twist, would have no strength at all.

The mechanics of fiber bundles was studied beginning from the first half of the twentieth century in connection with developments in the textile industry and continues today with the development of stochastic models of failure in bundles with and without an embedding matrix, of importance in composites and biological applications. Several central results from this broad literature are summarized in this section. We begin by discussing the axial and bending deformation of bundles of continuous
fibers of the type shown in Figure 2.22(a). Further, results on the structure and tensile response of twisted bundles of the type shown in Figure 2.22(c) are presented. The strength of bundles of continuous and discontinuous fibers is also discussed.

2.5.1 The Deformation of Bundles of Continuous Fibers

2.5.1.1 Axial Deformation

When bundles of continuous parallel and straight fibers are loaded axially, all fibers experience the same strain. Hence, the bundle inherits the axial behavior of individual fibers. If these are elastic, the effective bundle modulus is given by:

$$E_{\text{eff}} = \langle E_f \rangle \phi_a,$$

(2.53)

where $\langle E_f \rangle$ is the mean Young’s modulus of individual fibers, while $\phi_a$ is the area fraction occupied by fibers in the bundle cross-section. The closest packed arrangement of fibers is hexagonal. In this case, and in the limit of large number of fibers in the bundle, $\phi_a = \frac{\pi}{2\sqrt{3}} \approx 0.9$. Equation (2.53) accounts for situations in which fibers have the same cross-sectional area but have different moduli.

In realistic bundles, fibers are not in the idealized close-packed hexagonal configuration. The free volume within bundles depends on the fabrication method. Further, the free volume changes with axial loading. The actual value of $\phi_a$ of a specific bundle can be evaluated by direct microscopic inspection.

2.5.1.2 Bending Deformation

The behavior of bundles subjected to bending is more complex and depends on the nature of the interfaces between fibers. Figure 2.23 shows several possibilities which are also extreme cases of behavior that may be encountered in practical situations.

Figure 2.23(a) shows a bundle in which inter-fiber interfaces are well bonded and are able to carry shear stress. The strong interfaces also prevent the rearrangement of fibers in the bundle during deformation. The figure shows the deformed configuration, with the bundle cross-section planes at A and B, which are taken perpendicular to the bundle axis before deformation, remaining perpendicular to the bundle axis after deformation.

![Figure 2.23](https://doi.org/10.1017/9781108779920.003) Fiber bundles subjected to bending (a) with axial constraint, (b) free to slide axially, and (c) with no constraint in the $x_2$ direction.
In this case, the bundle bends as a beam of effective moment of inertia, \(I_{\text{eff}}\), and the deformation can be described with elementary beam theory. The effective moment of inertia depends on fiber packing. In the limit of large number of fibers in the bundle, \(n_f\), and for close-packed fiber arrangement, the effective moment of inertia is given by \(I_{\text{eff}} \sim n_f^2 I_f\). If fibers are more sparsely packed, \(I_{\text{eff}}\) increases with decreasing \(\phi_a\).

Figure 2.23(b) shows another limit case, in which inter-fiber interfaces are weak and allow relative sliding. However, the packing is dense enough to prevent fiber rearrangement within the bundle during deformation. In this case, each fiber bends about its own centroidal axis. In this configuration, the fibers act as independent springs loaded in parallel and \(I_{\text{eff}} \sim n I_f\). This bundle has much smaller rigidity compared to the bundle with strong interfaces shown in Figure 2.23(a).

A situation encountered often in practice is that in which the bundle density is low and fiber packing is insufficient to prevent fiber migration and rearrangement within the bundle during bending. In this case, the cross-section of the bundle changes along the bundle length, becoming flatter in the center. This case is shown schematically in Figure 2.23(c).

To reduce complexity, we treat this case under the assumption that fibers are pin-jointed at their ends A and B and hence carry only axial forces. The cross-sections at A and B are given rotations of angles \(\theta/2\) and \(-\theta/2\), respectively (pure bending of the bundle). Therefore, the fibers above the median plane of the bundle (i.e., the plane defined by the axes of rotation of sections A and B) are subjected to tension and remain straight, while the fibers below the bundle median plane are subjected to compression and buckle, as shown in Figure 2.23(c). This motion leads to the increase of the fiber density in the middle cross-section of the bundle. The maximum deflection of a fiber located at distance \(r\) from the median plane of the bundle, \(w\), is given by:

\[
\left(\frac{w}{L_0}\right)^2 = \left(\frac{2}{\pi}\right)^2 \frac{r^2 \theta}{L_0} \left(1 - \frac{r \theta}{L_0}\right),
\]

(2.54)

where all lengths are normalized by the undeformed bundle length, \(L_0\). The position in the \(x_2\) direction of a fiber located above the bundle median plane shifts down by \(r(1 - \cos \theta/2)\). A fiber located below the bundle median plane shifts up by the same amount and also bends up. The maximum displacement in the \(x_2\) direction is \(w + r(1 - \cos \theta/2)\) and corresponds to the mid-span point of the respective fiber. Therefore, the density of fibers increases close to the median plane of the bundle and the bundle cross-section flattens out, expanding in the plane perpendicular to the \(x_2\) axis (Figure 2.23(c)).

### 2.5.2 Structure and Mechanics of Twisted Fiber Bundles

#### 2.5.2.1 Structure of Twisted Bundles

The twisting of fiber bundles has complex mechanics and leads to significant modifications of the bundle structure. This procedure is used with virtually all textiles; twist is applied with concomitant stretching of the yarn. Several methods to produce twisted
yarn have been developed, with ring spinning being the oldest method and the procedure that leads to the highest strength and quality of the yarn. The relatively low productivity of ring spinning led to the development of newer techniques such as rotor spinning and air jet spinning. This section presents a simplified description of yarn spinning aimed to outline the complexities that arise in this problem. The structure described here is characteristic primarily for the ring spinning method, while some variations are introduced by the other methods.

Figure 2.24(a) represents an idealized situation in which initially straight fibers parallel to the bundle axis become helices in the twisted configuration. The initial length of the bundle and of all its fibers is \( L_0 \), while the final length of the bundle corresponding to one full turn is denoted by \( L \). Figure 2.24(b) shows the unwrapped cylindrical surface containing a helical fiber at distance \( r \) from the bundle axis and the outer surface of the bundle. The length of the fiber wrapped around the cylinder of radius \( r \) is:

\[
l(r) = \sqrt{L^2 + (2\pi r)^2}.
\]

The angle of the fiber axis with the bundle axis is \( \alpha(r) \), which takes the value \( \alpha^* \) for \( r = R \). Hence, \( l \in (L, L/\cos \alpha^*) \) and the mean fiber length can be evaluated as:

\[
\langle l \rangle = \frac{L}{2} \left( 1 + \frac{1}{\cos \alpha^*} \right).
\]

The rather restrictive assumptions about the fiber kinematics made here imply that all fibers deform by stretching. Since this is an energetically expensive deformation

\[\text{Figure 2.24 (a) Bundle of fibers initially parallel to the bundle axis subjected to twisting, under the assumption that fibers initially at distance } r \text{ from the bundle axis are constrained to wrap on the surface of the cylinder of radius } r. \text{ One full turn of two such fibers wrapping on cylinders of radii } r \text{ and } R \text{ is shown. (b) Unwrapped cylinders of radii } r \text{ and } R \text{ of the deformed configuration showing the two spiral fibers represented in (a), which become straight lines in this representation.}\]
mode, the bundle tends to reduce its length to release some of the axial fiber strain. One may envision that the real deformation is such that

$$\langle l \rangle = L_0.$$  \hspace{1cm} (2.57)

This implies that fibers close to the bundle axis are compressed and buckle, while those close to the outer layers of the bundle are stretched. Replacing $\langle l \rangle$ of Eq. (2.57) in Eq. (2.56) and assuming that the mean bundle density remains constant during deformation, such that $\pi R^2 L = \pi R_0^2 L_0$, allows computing of the length of the bundle, $L$, characterized by the twist of angle $\alpha^*$ on the outer surface:

$$\frac{L}{L_0} = \frac{1}{2} \left( 1 + \sqrt{1 - \frac{4\pi^2 R_0^2}{L_0^2}} \right),$$ \hspace{1cm} (2.58)

$R_0$ represents the radius of the bundle of straight fibers before twisting and it is implied that the radius of the bundle increases during twisting since its length decreases.

Equation (2.58) can be used to compute the axial contraction strain of the bundle due to the twist, that is, $(L_0 - L)/L_0$. For small values of the twist (i.e., for small $R_0/L_0$), this contraction strain can be approximated to the first order as:

$$\frac{L_0 - L}{L_0} \approx \pi^2 R_0^2 \frac{L_0^2}{L_0^2},$$ \hspace{1cm} (2.59)

which indicates that the contraction decreases quadratically as the length of the bundle corresponding to one turn, $L_0$, increases. The characteristic angle $\alpha^*$ decreases in this process. Figure 2.25 shows experimental data for the contraction strain in twisted cotton yarn (Landstreet et al., 1957). The data indicates that the axial strain scales with $L_0$ as $(L_0 - L)/L_0 \sim L_0^{-1.66}$. The difference relative to the prediction of Eq. (2.59) is due to the multiple assumptions made in this simplified model, of which the most

![Figure 2.25](https://doi.org/10.1017/9781108779920.003) Axial strain of a fiber bundle function of the twist (proportional to $1/L_0$) for cotton yarn. The horizontal axis represents the inverse axial length corresponding to one turn. Data from Landstreet et al. (1957)
important is related to the structure of the twisted bundle. The consequences of relaxing these assumptions are discussed next.

The arrangement of fibers in a twisted bundle was studied in detail by Morton (1956), Riding (1964), Treloar (1965), and Hearle et al. (1969). In 1956, Morton proposed that fibers migrate in the radial direction as the bundle is twisted (Morton, 1956). The main argument is geometric: since fibers closer to the axis of the twisted bundle must contract relative to their initial length, $L_0$, and since axial compressive strains are not supported by thin fibers, these fibers must accumulate slack.

A similar argument can be made based on energetic considerations: the axial deformation mode is energetically expensive and fibers should deform preferentially in the much softer bending mode. This implies that fibers on the outside of the bundle should seek to move closer to the axis of the bundle, while those initially closer to the axis should seek trajectories that move outward in order to keep the bundle density approximately constant and minimize the total strain energy.

This fiber arrangement is, indeed, observed in most twisted bundles and yarns. Figure 2.26 shows experimental data reported in Riding (1964). The curve shows the radial position of a tracer fiber in a twisted bundle along the bundle axis. At the left end of the trace, this fiber is closer to the bundle surface, but it migrates toward the bundle axis. A radial migration pattern, in and out, is observed, with a periodicity of about 4 mm. The periodicity depends on the density of the bundle and on whether twisting is applied with a superimposed stretch or not.

Fiber migration is controlled by packing and energetics. Fibers tend to migrate in order to reduce their axial strain and stored strain energy. However, migration is difficult in a densely packed bundle. The interplay of these mechanisms was studied and an instructive review is presented in Hearle et al. (1969), while a more recent account can be found in Neckar and Das (2018). The situation is qualitatively illustrated in Figure 2.27, which shows the frequency of radial fiber migration in the bundle function of the tension applied during twisting. If the bundle is not stretched, the bundle diameter increases upon twisting, the inner fibers accumulate slack and tend to move outward, while the outer fibers are stretched and tend to move inward.

![Figure 2.26](https://doi.org/10.1017/9781108779920.003) Radial position of a tracer fiber in a twisted bundle function of position along the bundle axis. Adapted from Riding (1964)
Radial migration is controlled by this energetic mechanism and fibers develop trajectories within the bundle which allow strain energy minimization. As tension increases, the bundle becomes more compact and the increased packing makes migration difficult. Two mechanisms cause increased packing: the reduction of slack of the central fibers due to the application of external axial loads, and the radial compressive force applied by helical fibers when subjected to a superposition of axial and torsion external loads. The result of the combination of these mechanisms is the continuously decreasing trend of fiber radial migration shown in Figure 2.27. These conclusions are supported by experimental observations with twisted textile yarns.

It is of interest to observe that as an initially straight fiber acquires a helical shape during bundle twisting, it is bent by a moment aligned to the bundle axis (i.e., by the bundle twisting moment). This moment, $M$, is shown schematically in Figure 2.24(b). Decomposing the moment in the direction perpendicular and parallel to the fiber axis, it results that fibers are both bent (by the component perpendicular to the fiber axis, $M_b$) and twisted (by the component aligned with the fiber axis, $M_t$). Fibers closer to the bundle axis are twisted more. This acquired chirality contributes to the inter-fiber load transfer via frictional forces.

2.5.2.2 Mechanical Behavior of Twisted Bundles
Twisted bundles, such as yarns used in the textile industry, twisted cables, and ropes, are mostly loaded in tension along the bundle axis. We focus here on this type of loading.

Twisting reduces the stiffness of the bundle. Consider that the bundle follows the affine kinematics and the strain on the scale of individual fibers is equal to the imposed axial, tensile strain applied to the bundle. Figure 2.28(a) shows the side view of a bundle subjected to an imposed axial strain $\varepsilon$ and a resultant force $P$. Figure 2.28(b) shows one of the fibers of the bundle which forms a helix characterized by the angle $\alpha(r)$. The fiber is strained axially by $\varepsilon_f(r) = \varepsilon \cos^2 \alpha(r)$, which leads to an axial force $P_f(r) = E_fA_f\varepsilon \cos^2 \alpha(r)$. This fiber contributes to the total axial force in the bundle with the projection of $P_f$ in the bundle axis direction, that is, $P_{f\|}(r) = E_fA_f\varepsilon \cos^2 \alpha(r)$. The total force in the bundle results by summing up these contributions:
\[ P = \int \int P_\parallel (r) \frac{\phi_a}{A_f / \cos \alpha(r)} r \, dr \, d\theta, \]  

(2.60)

where \( \phi_a \) represents the area fraction of fibers in the untwisted bundle, while the ratio under the integral represents the area fraction in the bundle cross-section at distance \( r \) from the bundle axis. Fibers close to the bundle axis are almost straight (small \( \alpha \)) and appear in the bundle cross-section as circles, while those at larger \( r \) appear as ellipses, as shown in Figure 2.28(c). The stiffness of the bundle is evaluated using Eq. (2.60) by dividing \( P \) by the area of the bundle and the imposed strain, \( \varepsilon \). It results that the bundle stiffness is \( E = E_f \phi_a \langle \cos^4 \alpha(r) \rangle \), where \( \langle \rangle \) represents averaging over the cross-section. Performing this average one obtains:

\[ E \sim E_f \phi_a \cos^2 \alpha^*. \]  

(2.61)

Figure 2.29 shows experimental data from yarns of various polymeric fibers twisted to different degrees (Hearle et al., 1959). The figure supports the scaling of the
modulus with the twist angle indicated by Eq. (2.61), especially at low twists. As the twist increases, fiber migration and the associated disordering of the bundle structure make the physical picture more complex and some departure from the prediction of Eq. (2.61) is observed.

Figure 2.30 shows load–elongation curves for bundles of continuous nylon fibers with 0, 30, and 70 turns per inch twist (Hearle et al., 1959). The two axes are normalized with the peak force and the elongation of the reference untwisted bundle. The decrease of the bundle stiffness with increasing twist is clearly visible. Further, rupture is more gradual in the untwisted bundle compared with the twisted bundles, which exhibit brittle failure. This is due to the inherent presence of some degree of tortuosity in the untwisted bundle. The tortuosity is eliminated as the degree of twist increases. Interestingly, it emerges that the failure stress is largely independent of the twist. The elongation at failure increases as twist increases due to the reduction of the effective bundle stiffness (Eq. (2.61)). These trends have been reported in the literature for different types of bundles.

The situation can be understood qualitatively starting from the following considerations. If the bundle is twisted without being subjected to a tensile force, the fibers close to the bundle axis acquire slack and migrate outward, potentially increasing the free volume of the bundle. The outer fibers are subjected to tension during twisting. If they deform plastically, the elastic rebound during unloading is insignificant, but these fibers have accumulated plastic strain and are closer to their failure strain. In this case, when subjected to subsequent axial testing (without increasing the twist), the outer fibers will break first. Hence, the failure strain should depend on the degree of twist. If fibers remain elastic, the rebound upon unloading is large and puts the fibers close to the bundle axis in compression, therefore increasing the slack. Upon loading, the middle fibers carry little load and, hence, in this case too, the outer fibers break first. This argument implies that the fraction of load bearing fibers decreases with increasing twist and hence the failure strain is expected to depend on the magnitude of twist.
If the bundle is twisted under axial load, slack is reduced. If fibers deform plastically, the elastic rebound is limited and no slack is introduced. Hence, the failure strain is expected to be independent of twist in this case. The situation is opposite if fibers deform elastically at all times. Real situations are in-between these extreme cases.

2.5.3 Bundles of Discontinuous Fibers: The Shear Lag Model

If fibers are discontinuous, the integrity of the bundle hinges on the existence of an appropriate inter-fiber load transfer mechanism. In biological materials and in textile yarns, fibers are of finite length and, in most cases, are much shorter than the length of the bundle. This is in contrast with the situation of structural fiber-reinforced composites and most nonwovens which are made from nominally continuous fibers.

Collagen fibers are bundles of fibrils which are cross-linked within the bundle. In textiles the fibers within yarns are not cross-linked but interact frictionally. Cotton and wool fibers have diameters of tens of micrometers and an aspect ratio larger than 1 000. Carbon nanotubes form bundles with cohesive inter-tube interactions, which is a rather weak load transfer mechanism. The tubes have nanometer cross-sectional dimensions and lengths as large as millimeters, so the aspect ratio can be as high as $10^6$.

Fiber–fiber interactions that may lead to effective load transfer include the cross-linking of fibers, inter-fiber friction, and adhesion. It is important in this context to analyze how loads are transmitted between fibers within the bundle. The answer is provided by the shear lag model developed in the literature related to composite materials (Cox, 1952) and subsequently used in other contexts for many material systems.

Consider the configuration in Figure 2.31(a), where two fibers are in contact along a segment of length $L$ and are loaded by a force $P$ which promotes relative sliding in the axial direction. The width of the contact surface is $2a_X$ (see Figure 3.4 for the definition of this parameter). The fiber material is considered linear elastic, of modulus $E_f$. The interface is subjected to shear (as stated, the problem is one-dimensional) and may be represented either with a continuum or a discrete model. In the continuum representation, an effective thickness, $h_X$, and a shear modulus, $G_X$, are assigned to the interface and load transmission is assumed to take place at all points of the contact area. In the discrete interface model, it is assumed that the two fibers are connected at discrete points by springs of stiffness $k_X$ separated in the axial direction by $l_X$. This representation is adequate for situations in which nanoscale fibers are crosslinked by fibrils of molecular strands (Figure 2.31).

The equilibrium condition for the fiber element of length $dx$ requires:

$$\frac{d\sigma_1}{dx} = -\frac{d\sigma_2}{dx} = \frac{2a_X}{A_f},$$

(2.62)

where $\sigma_1$ and $\sigma_2$ represent the axial stresses in the two fibers. The constitutive equation of fibers reads:

$$\sigma_i = E_f \frac{du_i}{dx}, \quad i = 1, 2.$$  

(2.63)
The continuum interface is described by

\[ \tau = \frac{G_X}{h_X} \left( u_1(x) - u_2(x) \right), \tag{2.64a} \]

while the discrete interface is described by

\[ \tau = \frac{k_X}{2a XL} (u_1(x) - u_2(x)), \tag{2.64b} \]

with the relation \( G_X = k_X h_X / 2a XL \) establishing the equivalence of the two models.

Noting that Eq. (2.64b) leads to:

\[ \frac{d\tau}{dx} = \frac{k_X}{2a XL E_f} (\sigma_1(x) - \sigma_2(x)), \tag{2.65} \]

the equilibrium equations (Eq. (2.62)) can be rewritten as:

\[ \frac{d^2 \sigma_1}{dx^2} = \frac{1}{\lambda_{sl}^2} (\sigma_1 - \sigma_2), \tag{2.66} \]

\[ \frac{d^2 \sigma_2}{dx^2} = \frac{1}{\lambda_{sl}^2} (\sigma_2 - \sigma_1), \tag{2.66} \]

where

Figure 2.31 (a) Problem set-up and stress distribution predicted by the shear lag model (Eq. (2.68)), for (b) \( \sqrt{2} \lambda_{sl}/L = 0.2 \) and (c) \( \sqrt{2} \lambda_{sl}/L = 1 \).
\[ \lambda_{sl} = \sqrt{\frac{E_f A_f h_X}{k_X}} = \sqrt{\frac{E_f A_f h_X}{G_X 2a_X}} \]  

(2.67)

is known as the shear lag length and is a characteristic length scale emerging from the mechanics of load transmission across the interface. This parameter represents the relative stiffness of the fibers and the interface and has large values when fibers are much stiffer than the interface and small values when fibers are compliant.

Equations (2.66) are solved with boundary conditions representing for each fiber the condition that the stress, \( P/A_f \), is imposed at one end, while the other end is traction free: \( \sigma_1(0) = 0 \), \( \sigma_1(L) = P/A_f \), \( \sigma_2(L) = 0 \), and \( \sigma_2(0) = P/A_f \). The solution reads:

\[
\sigma_1(x) = \frac{P}{A_f} \sinh \frac{x/L}{\sqrt{2\lambda_{sl}}/L} \cosh \frac{1 - x/L}{\sqrt{2\lambda_{sl}}/L} \\
\sigma_2(x) = \sigma_1(L - x) \\
\tau(x) = \frac{P}{2\sqrt{2a_X\lambda_{sl}}} \cosh \frac{2x/L - 1}{\sqrt{2\lambda_{sl}}/L} \sinh \frac{1}{\sqrt{2\lambda_{sl}}/L} 
\]  

(2.68)

The solution of Eq. (2.68) is graphically presented in Figure 2.31(b) and (c) for two values of the shear lag parameter, \( \sqrt{2\lambda_{sl}}/L \). In the compliant fibers case, when the shear lag length is small, \( \lambda_{sl} \ll L \), the interface is loaded only in a region close to the two fiber ends, of length approximately equal to \( \lambda_{sl} \), as shown in Figure 2.31(b). The interface carries no loads in the central part of the fiber. Consequently, the axial stress is constant in the central section of the fiber and varies close to the fiber ends. The opposite situation is obtained as the fibers become stiffer and \( \lambda_{sl} \) increases: the region of load transmission extends along the interface and, in the limit of rigid fibers and very large \( \lambda_{sl} \), load is transmitted uniformly along the interface and the axial stress in fibers varies linearly, as shown in Figure 2.31(c). Since fibers slide as rigid bodies in this case, the relative slip is constant along the interface.

### 2.5.4 Failure of Bundles of Continuous and Discontinuous Fibers

The failure of fiber bundles of continuous and discontinuous fibers subjected to uniaxial tension is discussed in this section. In the case of discontinuous fiber bundles, load transfer between fibers is necessary in order to ensure the integrity and load carrying capacity of the bundle. Load transfer occurs via intra-bundle crosslinks or through the matrix that embeds the fibers, if present.

Bundles of continuous fibers may carry loads in the absence of intra-bundle crosslinks. In this case, rupture of a fiber leads to the redistribution of the load to the remaining intact fibers. Load redistribution may take place equally to all remaining
fibers of the bundle, or exclusively to the neighbors of the broken fiber. The exact load redistribution modality is generally unknown and many models have been proposed in the literature addressing this problem. Reviews of fiber bundle models are presented in Phoenix (1993) and Pradhan et al. (2010). It should be noted that a continuous fiber bundle with an inter-fiber load transfer mechanism becomes similar to a discontinuous fiber bundle once the fibers start failing. This is because a fiber that breaks can still carry loads at distances along the respective fiber from the rupture site larger than $\lambda_{sl}$, provided a mechanism which transfers load from the neighboring fibers operates. Hence, any fiber of the bundle may experience rupture at multiple sites and become fragmented, entailing that the bundle becomes similar to a discontinuous fiber bundle with stochastic fiber lengths.

Due to its prevalence, we focus here on the failure of discontinuous fiber bundles, an example of which is shown schematically in Figure 2.32. It is considered that fibers are connected by inter-fiber crosslinks which behave as linear springs of stiffness $k$ (per unit length of contact) – a situation similar to that discussed in Section 2.5.3 in the context of the shear lag model. Crosslinks are thought to be uniformly distributed in the interface between any two fibers in contact. For simplicity, it is assumed that fibers have identical length, $L$, and any fiber row in the bundle is shifted relative to its neighbors by a random distance (Figure 2.32).

Loads are transmitted from fiber to fiber across interfaces. If the shear lag length $\lambda_{sl}$ is much smaller than $L$, the loads are transmitted between fibers in the vicinity of fiber ends. The bundle may fail by the rupture of fibers only, the rupture of crosslinks only, or by the rupture of both fibers and crosslinks. If fibers do not break, failure takes place along interfaces, followed by fiber pull-out. The bundle ruptures in this case along the shortest path across the bundle running along interfaces, as shown in Figure 2.32. The energy dissipated in this process depends on the length of this path; this failure mode provides the largest toughness of all three failure modes mentioned here. If interface failure does not take place and the bundle ruptures exclusively by the failure of fibers, the only possibility is for all fibers in a given cross-section to fail, which implies that a major crack cuts across the bundle leading to brittle failure. The intermediate case, in which both fibers and interfaces fail, requires fiber pull-out to an extent smaller than that of the situation shown in Figure 2.32. The associated toughness is also intermediate between the other two cases.

This qualitative discussion suggests that the behavior may be described in terms of two non-dimensional parameters: the ratio of the fiber strength to the crosslinks strength, $\sigma_f^b/\sigma_X$, and the ratio of the fiber length to the shear lag length, $L/\lambda_{sl}$.

![Figure 2.32](https://doi.org/10.1017/9781108779920.003) Schematic showing the localization of relative fiber sliding leading to bundle rupture. The dashed line shows the localization path.
Figure 2.33 shows the expected deformation and failure modes in the space of these two parameters. Based on the results of the shear lag analysis of Section 2.5.3, at large values of $L/\lambda_{sl}$ load transfer is localized at the ends of fibers, while at small values of this parameter load transfer is distributed over larger lengths of the interfaces, starting from fiber ends. If the crosslinks are weaker than the fibers, that is, $\sigma_f^c/\sigma_X^c \gg 1$, bundle failure takes place mainly along interfaces and involves fiber pull-out. If interfaces are strong and fibers have low strength, bundles fail due to fiber rupture. The load transfer mechanism makes a difference in this case: at large values of $L/\lambda_{sl}$, when load transfer is localized, fibers carry approximately constant load along segments defined by the position of fiber ends of neighboring fibers. In the low $L/\lambda_{sl}$ case, the axial force varies continuously along the length of fibers. If fibers have stochastic strength, the probability that a fiber ruptures at multiple sites along its length is lower in the low $L/\lambda_{sl}$ case than in the high $L/\lambda_{sl}$ case. Hence, moving from left to right along the horizontal axis at low values of the ordinate, it is expected that bundle failure becomes more localized. The bundle toughness should increase with increasing $\sigma_f^c/\sigma_X^c$ due to the change of the failure mode from localized fiber failure to gradual pull-out.

As discussed in Section 2.3.7, in most situations of practical interest the strength of fibers is stochastic and varies along their length. This is particularly important in the case of long, continuous fibers such as those used in structural composites. The fiber strength is generally described by the weakest link theory, which leads to the Weibull statistics. Equation (2.11) provides the cumulative probability that a fiber fails at a stress smaller than $\sigma$, $cp_f(\sigma) = 1 - \exp \left( -\sigma/\sigma_0^\beta \right)$, with $\beta$ and $\sigma_0$ being the Weibull modulus and the scale factor of the distribution.

In the context of the present discussion, it is of interest to investigate the functional form of the failure probability of the fiber bundle, $cp_b(\sigma)$, given that the individual fiber strength is described by Weibull statistics, $cp_f(\sigma)$. The answer to this question is sought in a vast literature on the “fiber bundle model” which was proposed about
100 years ago in the literature on textile fibers and is still being used in statistical physics for problems such as the occurrence of avalanches and failure of brittle solids. As briefly discussed at the beginning of this section, the basic model assumes that the behavior of all fibers is elastic up to a value of the stress at which failure occurs, after which the load carried by the respective fiber is redistributed to the fibers which are still intact. Models of this type differ with respect to the assumptions regarding load redistribution. Many refinements have been proposed, including accounting for time dependence (Newman and Phoenix, 2001), the hierarchical organization of bundles (Pimenta and Pinho, 2013), fiber and crosslink strength distributions (Swolfs et al., 2015; Kádár et al., 2017), etc. Such models have been applied to a broad range of fibrous systems such as carbon nanotube bundles (Zhang et al., 2014), silk (Bosia et al., 2010), and unidirectional fiber composites (Okabe et al., 2005; Bunsell et al., 2018), and to the failure of nonfibrous materials such as bone and nacre (Zhang et al., 2010). A review of these works with a statistical physics flavor is presented in Pradhan et al. (2010).

To demonstrate the general behavior in the context of the bundle model used in the present section (Figure 2.32), consider first bundles with \( \sigma^c_D = 0.05 \) in which the mean of the strength distribution of fibers, \( \sigma^c_f \), is 20 times smaller than the (deterministic) strength of inter-fiber crosslinks. In this case, fibers fail first and bundle failure is localized. Figure 2.34(a) shows the cumulative distribution of bundle failure along with the corresponding distribution of fiber failure, which is an input to the model. The mean bundle strength, \( \langle \sigma^b \rangle \), is somewhat smaller (but comparable to) than the mean fiber strength. However, the more obvious effect is the drastic increase of the Weibull modulus when going from the fiber to the bundle scale. This implies that the variability of the bundle strength is much smaller than that of the individual fiber strength.

Figure 2.34(b) shows a similar result for the bundle with \( \sigma^c_D = 5 \), in which failure is controlled by crosslink rupture and fiber pull-out. The mean bundle strength is significantly smaller than the mean fiber strength, which is a consequence of the fact that bundle failure is related to interface failure. In this case too, the bundle strength variability is much smaller than the variability of the fiber strength.

The functional form of the emerging bundle strength distribution, \( c_{pb}(\sigma) \), cannot be derived, except in a few cases in which the bundle model can be solved analytically. The first such model is due to Daniels (1945) and considers bundles of continuous fibers with no inter-fiber load transmission and equal load sharing among the fibers that remain intact. In this case, the bundle strength follows a Gaussian distribution, with variability decreasing inversely as the square root of the number of fibers in the bundle. Following the work of Daniels, Coleman (1958) derived the mean strength of a bundle of continuous fibers of the same constitutive behavior, but with strengths described by a Weibull distribution of Weibull modulus \( \beta \) (Eq. (2.11)). The analysis is performed under the assumption of equal load sharing, in which all remaining fibers in the bundle share equally the load carried by fibers that break. Coleman’s analysis indicates that the mean bundle strength, \( \langle \sigma^b \rangle \), is smaller than the mean fiber strength, \( \langle \sigma^c_f \rangle \), and the ratio of these two quantities is described by:
where $\Gamma$ represents the Gamma function. This ratio is a function of the Weibull modulus of the fiber strength distribution only and decreases continuously with decreasing $\beta$, that is, with increasing fiber strength variability. Figure 2.34(c) shows the variation of $\langle \sigma_b^\prime \rangle / \langle \sigma_f^\prime \rangle$ with the coefficient of variation of the fiber strength distribution $cp_f(\sigma)$ (the coefficient of variation of the Weibull distribution can be approximated as $1/\beta$).

Other analytic and numerical results for the statistics of bundle strength under various types of load redistribution and inter-fiber load transmission are summarized in a review article (Phoenix and Beyerlein, 2000).

The strength of bundles of discontinuous fibers with twist is of great interest in textiles. The mechanism that allows ropes to acquire strengths larger than that of individual fibers is based on the interplay of friction and twist.
A bundle of discontinuous fibers in which the only inter-fiber load transfer mechanism is frictional has no strength if fibers are straight, since no normal forces that may engage friction act between parallel fibers loaded axially. For inter-fiber friction to be engaged, the bundle must be twisted. With an ideal twisting pattern, as shown in Figure 2.24, which requires that fibers become helical and preserve their distance to the bundle axis, it is clear that inter-fiber friction is not engaged. Two features lead to the desired effect: (i) the fact that a helical fiber loaded in tension along the axis of the helix tends to move inward, reducing the radius of the respective helix, and (ii) twist-induced fiber migration. The first mechanism creates radial forces compressing the central region of the bundle, while the second mechanism allows fibers on the outside of the bundle to visit the bundle core, and hence become frictionally engaged with the other fibers. This implies that load transfer takes place when a fiber traverses the core of the bundle, while the other segments of the respective fiber, which are located farther from the bundle axis, carry constant axial force. For the mechanism to be effective with staple fibers, the fiber length must be larger than the distance along a given fiber between segments that traverse the bundle core (Figure 2.26).

The bundle strength is limited at low twists by the weak load transfer, since fibers are approximately parallel to the bundle axis and fiber migration is negligible. Under such conditions, the load carried by individual fibers is small and bundle failure takes place primarily by fiber pull-out. At high degrees of twist leading to pronounced fiber migration, load transfer is efficient and strength is controlled by fiber rupture. Overall, the strength versus twist curve is defined by the dependence of the load transfer mechanism and of the stress carried by fibers on the degree of twist. Figure 2.35(a) shows these trends schematically. Load transfer becomes more efficient with increasing twist and this leads to the increase of the bundle strength, as shown by curve AB. The strength of individual fibers limits the bundle strength at large degrees of twist, as shown schematically by curve CD. This decreasing trend can be understood based on the analysis of the simplified bundle model leading to Eq. (2.61). Specifically, in this

![Figure 2.35](https://doi.org/10.1017/9781108779920.003) Variation of the bundle strength with the angle of twist: (a) schematic representation of trends, and (b) experimental data obtained with cotton yarns. Data from Landstreet et al. (1957)
model, the stress carried by the bundle, \( \sigma \), is related to the strain on the bundle scale, \( \varepsilon \), as
\[
\sigma = E_f \phi_a \varepsilon \cos^2 \alpha^* \quad \text{(see Eq. (2.61))},
\]
and \( \varepsilon \) is related to the axial strain in the fiber located at distance \( r \) from the bundle axis and forming a helix of angle \( \alpha(r) \) by
\[
\varepsilon_f(r) = \varepsilon \cos^2 \alpha(r).
\]
Since the stress in the fiber is \( \sigma_f(r) = E_f \varepsilon_f(r) \), the stress in the fiber and the bundle-scale stress are related as
\[
\sigma = \sigma_f(r) \phi_a \cos^2 \alpha^* / \cos^2 \alpha(r). \quad \text{(In this simplified model, the fibers close to the bundle axis are the most loaded. Requiring that for these fibers \( \sigma_f(r) = \sigma_f \), where \( \sigma_f \) is the fiber strength, it results that the bundle strength, \( \sigma_c \), scales as \( \sigma_c \sim \cos^2 \alpha^* \). This equation quantifies the decreasing trend of curve CD in Figure 2.35(a). The actual dependence of the bundle strength on the twist is the combination of the two aforementioned trends and exhibits a non-monotonic behavior and the emergence of an optimal value of twist corresponding to the position of the maximum strength (Figure 2.35(a)). Figure 2.35(b) shows experimental data obtained with cotton yarns of various degrees of twist (Landstreet et al., 1957) confirming the trends discussed here.)

Predicting the optimal twist \( \alpha^*_0 \) of a fiber bundle is of practical importance. Here it suffices to observe that the position of the peak in Figure 2.35(a) can be adjusted by controlling the rate at which curve AB increases. If twist enables the load transfer mechanism efficiently, AB increases faster with \( \alpha^* \), and consequently \( \alpha^*_0 \) decreases. This can be achieved by increasing the fiber length and increasing the inter-fiber friction coefficient. Both of these variables have been observed experimentally to reduce the value of the optimal bundle twist.

A number of refinements can be made to this physical picture by taking into account fiber migration, the details of load transfer in view of the shear lag mechanism, the dependence of the fiber strength on fiber length, etc. The reader is referred to the relevant literature for a review of these effects (Hearle et al., 1969; Neckar and Das, 2018).

References


