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Mechanical modeling of rheometer experiments: Applications to rubber and actin networks

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ABSTRACT

Experiments on cross-linked actin networks in form of a circular cylinder conducted with a rheometer and parallel-plate geometry resemble a torsional problem of a cylinder undergoing large deformation. A commonly used approximation for the analysis of such experiments is simple shear which is inappropriate for the global analysis of the more complex 3D torsion deformation. We compare the solutions of the torsion of a cylinder with simple shear on the basis of three (phenomenological) rubber models and two network models for cross-linked actin. We start with rubber elasticity and show that the approximation for materials with linear shear elasticity may be reasonable. In the case of cross-linked actin networks, however, the strong strain-stiffening behavior causes higher deviations of simple shear from the more realistic torsional mode. Furthermore, we show that the frequently used eight-chain model cannot account for the correct normal stress behavior of cross-linked actin networks. A recently proposed affine network model reproduces the correct sign for the normal stress for both versions of the boundary conditions. The two solutions, however, differ significantly so that an approximation of the deformation mode in a parallel-plate rheometer by simple shear should be used with caution.

1. Introduction

Rotational rheology with a parallel-plate geometry is the state-of-the-art experimental method for the mechanical characterization of materials such as (cross-linked) actin networks. The deformation of the samples in such experiments resembles the torsion of a cylinder. In several previous studies, however, simple shear was used as an approximation for the real situation in parallel-plate rheometry, see, e.g., [1–3]. One aim of the present study is to analyze and quantify this commonly used approximation.

During experiments with a parallel-plate rheometer and plate radius R the axial force $\tilde{N}$ and the applied torsion couple $\tilde{M}_{\mathrm{t}}$ are recorded and transformed into a normal stress component $\tilde{\sigma}$ and a shear stress component $\tilde{\tau}$, respectively. Thus [4],

$$\tilde{\sigma}=\frac{\tilde{N}}{\pi R^{2}},\quad \tilde{\tau}=\frac{2\tilde{M}_{\mathrm{t}}}{\pi R^{3}},\tag{1}$$

where the superimposed tilde is used to identify the values obtained from experimental tests.

Torsion of a cylinder undergoing large deformations in the context of rubber elasticity was solved in the seminal paper series on 'large elastic deformations of isotropic materials' by Rivlin, see, e.g., [5] and it was later discussed by Truesdell and Noll [6]. Torsion couple and axial force for the well-known neo-Hookean and Mooney–Rivlin models are also established in several text books, see, e.g., [4]. Refined models for rubber, for example the Yeoh model [7], may account for material non-linearities of rubber.

In the case of cross-linked actin networks we basically distinguish two modeling approaches. First, discrete models [8–12] are used to investigate the mechanics of a network on the filament scale. They are, however, expensive in terms of computational cost and, therefore, in general, only simple shear of a representative volume is considered. The second modeling approach aims for microstructurally motivated continuum models [1–3,13]. This approach models the properties of a single actin filament first to obtain a force–stretch relationship. Based on that, a network model is then employed to homogenize the discrete microstructure. In our study the parameters of the resulting continuum mechanical constitutive model are interpretable as the properties of the single filaments *and* the network topology.

In the present study, we show that simple shear may be used for certain types of material models to investigate the torsional response. Furthermore, we show that by using an affine network model for capturing the mechanical response of cross-linked actin networks, we obtain a tensile normal stress (also for the simple shear case) which is in accordance with, e.g., [14]. On the other

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hand, the eight-chain model is not able to generate tensile normal stresses. Subsequently, we distinguish three types of notation: (i) the tilde $(\tilde{\bullet})$ indicates rheological experiments with its measures as in (1), (ii) the hat $(\hat{\bullet})$ characterizes values which are related to simple shear, while (iii) no specific symbol refers to the torsion of a cylinder.

Section 2 establishes the governing equations for the torsion of a cylinder and conducts a comparison to simple shear. Subsequently, in Section 3, we apply the findings to material models for rubber and define related error measures. In Section 4 we focus on models for cross-linked actin networks. Specifically, we investigate an eight-chain model and an affine constitutive model for cross-linked F-actin networks. In the final Section 5 we provide a discussion and conclude the study.

2. Analytical solution of the torsion of a cylinder

In this section we briefly review the necessary kinematics required for the analysis of the torsion of a cylinder at finite strains. We introduce the most general form of the stress relation together with simple shear as a local approximation of simple torsion. Subsequently, we specialize these relations to materials which can be described in terms of strain invariants.

2.1. Non-linear continuum mechanics

Consider an incompressible circular cylinder with radius R and height Z in cylindrical polar coordinates (r, ϕ, z), as depicted in Fig. 1. A point in the reference and the current configuration are characterized by the position vectors $\mathbf{X}$ and $\mathbf{x}$, respectively. The index zero is employed to note the coordinates in the reference configuration, i.e. (r_0, ϕ_0, z_0). Hence, we describe the deformation through

$$r = r_0, \quad \phi = \phi_0 + kz_0, \quad z = z_0, \tag{2}$$

where k is the twist, with the unit m^{-1}. The angle Φ by which the top surface is rotated with respect to the bottom surface is $\Phi = kZ$. Hence, the deformation gradient $\mathbf{F}$ is given in the matrix form as

$$[\mathbf{F}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & kr \\ 0 & 0 & 1 \end{bmatrix}, \tag{3}$$

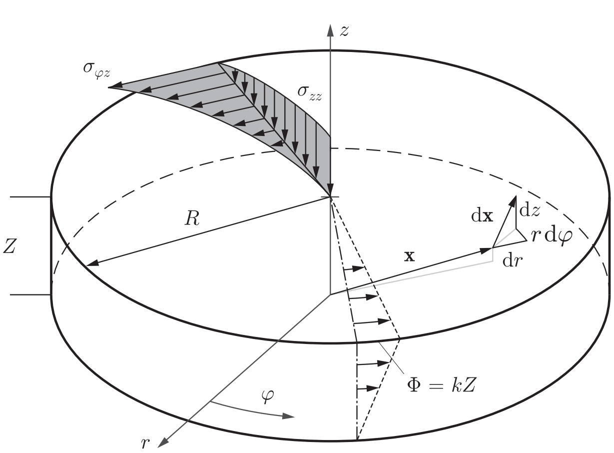

Fig. 1. Cylinder under torsion (dimensions R and Z) with a cylindrical coordinate system (r, ϕ, z). The components of the tangent vector $\mathrm{d}\mathbf{x}$ associated with the position vector $\mathbf{x}$are $\mathrm{d}r$, $\mathrm{d}\phi$ and $\mathrm{d}z$. The dash-dotted lines on the cylinder in the reference configuration deform to the dotted lines in the current configuration. The angle of rotation is $\Phi = kZ$, defined through the twist k. The gray areas schematically represent the distributions of shear stress $\sigma_{\phi z}$ and normal stress σ_{zz} over the radius r.

representing the linear transformation of a tangent vector $\mathrm{d}\mathbf{X}$ in the reference configuration to the current configuration $\mathrm{d}\mathbf{x}$, i.e. $\mathrm{d}\mathbf{x} = \mathbf{F}\,\mathrm{d}\mathbf{X}$. The first invariant $I_1 = \mathrm{tr}\,\mathbf{C}$ of the right Cauchy–Green tensor $\mathbf{C} = \mathbf{F}^\top \mathbf{F}$ is

$$I_1 = k^2 r^2 + 3. \tag{4}$$

Note that $J = \det \mathbf{F} = 1$, characterizing a volume-preserving deformation.

Assume now that the constitutive relation of the material can be expressed by the strain–energy function $\Psi(\mathbf{C})$ in terms of the right Cauchy–Green tensor. The Cauchy stress tensor $\boldsymbol{\sigma}$ is then given as

$$\boldsymbol{\sigma} = \overline{\boldsymbol{\sigma}} - p\mathbf{I}, \tag{5}$$

where $\overline{\boldsymbol{\sigma}} = 2\mathbf{F}(\partial\Psi/\partial\mathbf{C})\mathbf{F}^\top$ and p is a Lagrange multiplier associated with the incompressibility constraint which can be interpreted as a hydrostatic pressure. Assuming a static problem and neglecting body forces, the key equation is then the equilibrium in the radial direction, i.e.

$$\frac{\mathrm{d}\sigma_{rr}}{\mathrm{d}r} + \frac{1}{r}(\sigma_{rr} - \sigma_{\phi\phi}) = 0. \tag{6}$$

The equations for the circumferential and the axial directions lead to the conclusion that p does not change through the sample thickness or in the circumferential direction, but only in the radial direction. The radial normal stress σ_{rr} on the side surface of the cylinder must vanish, leading to the boundary condition

$$\sigma_{rr}|_{r=R} = 0. \tag{7}$$

Then, by using (5) in (6) and subsequent integration we obtain

$$p = \overline{\sigma}_{rr} + \int_R^r (\overline{\sigma}_{rr} - \overline{\sigma}_{\phi\phi}) \frac{\mathrm{d}r^\star}{r^\star} \tag{8}$$

for the hydrostatic pressure. This equation combines the equilibrium equation with the boundary condition, and hence all components of (5) are determined.

When conducting an experiment, as illustrated in Fig. 1, we rotate the top plate with respect to the bottom one by an angle Φ while holding the distance Z between the plates constant. Simultaneously we measure the torsion couple M_t applied to the sample and the required axial force N to keep the distance between the plates constant. The axial force N is simply given by

$$N = \int_A \sigma_{zz}\,\mathrm{d}A, \tag{9}$$

where A is the top surface of the cylinder. The torsion couple M_t is obtained by integration of the shear stress, which is the force per deformed area, multiplied by the lever r, i.e.

$$M_\mathrm{t} = \int_A r\sigma_{\phi z}\,\mathrm{d}A. \tag{10}$$

Note that for the cylinder $\mathrm{d}A = r\,\mathrm{d}r\,\mathrm{d}\phi$, with $\phi \in [0, 2\pi]$ and $r \in [0, R]$. A conversion to the equivalent stress components, analogous to (1), may be applied. Thus

$$\sigma = \frac{N}{\pi R^2}, \quad \tau = \frac{2M_\mathrm{t}}{\pi R^3} \tag{11}$$

are the related normal stress and shear stress components, respectively.

2.2. Simple shear as a local approximation

Simple shear may be seen as a local approximation of simple torsion of a circular cylinder since the torsion deformation of the 3D surface of a cylinder can be reduced to a plane simple shear deformation in the local neighborhood of a point. More precisely, it is the solution at the outer surface $r=R$ of the cylinder.