A stochastic model of stroma: interweaving variability and compressed fibril exclusion

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Abstract

Hyperelastic constitutive models of the human stroma accounting for the stochastic architecture of the collagen fibrils and particularly suitable for computational applications are discussed. The material is conceived as a composite where a soft ground matrix is embedded with collagen fibrils characterized by non-homogeneous spatial distributions typical of reinforcing stromal lamellae. A multivariate probability density function of the spatial distribution of the fibril orientation is used in the formulation of the lamellar branching observed on the anterior third of the stroma, selectively excluding the contribution of compressed fibrils. The physical reliability and the computational robustness of the model are enhanced by the adoption of a second order statistics approximation of the average structure tensors typically employed in fiber reinforced models.

Keywords: compressive fibril exclusion, hyperelasticity, lamellar branching, second order structure tensors

1. Introduction

The cornea is the external lens of the eye and carries out concerted protective, structural, and refractive functions. Since the cornea provides one-third of the total
refractive power of the eye and due to its accessibility, it stands as the privileged site for surgical interventions to correct conditions such as myopia, presbyopia, and astigmatism. Corneal refractive surgery demands accurate diagnostic and surgical plans, but the outcomes are not always optimal. Advanced numerical models of the cornea have been developed in recent years with the aim of supporting refractive surgery, although they are still far to be an active part of the current clinical practice since they fail to be patient-specific models. Indeed, patient-specific models derive only from the combination of advanced diagnostic imaging, correct interpretation of optical and mechanical experimental observations, and efficient computational models. For one, the interpretation of the most promising in-vivo dynamical test (contactless air-puff tonometer) calls for the description of features of the stromal tissue that are not of relevance under more traditional quasistatic loading. The present study is thus concerned with the definition of accurate material models of the stromal tissue, based on the description of the collagen fibril architecture according to its statistical distribution, characterized by a different degree of interweaving across the thickness and inactivity of the fibrils under compressive loading. Starting from a second order approximation of the strain energy density of a statistical distribution of collagen fibrils, a multivariate probability density function (PDF) is introduced to incorporate recent experimental data.

2. Hyperelastic fibril distributed models

2.1. Second order structure tensor approach
Stochastic models for fiber reinforced tissues derive from the seminal work of Lanir, where the contribution of fiber orientation to the mechanical response of soft tissues is formulated from a theoretical point of view. The computational challenge of describing the microstructural properties in a reliable manner motivated the development of several approximations. The present study departs from the second order approximation of the strain energy density \( \psi_f \) of the collagen fiber distribution illustrated in Pandolfi and Vasta. The approximation is based on the second order Taylor expansion of the strain energy density \( \psi_f \) of the collagen fiber distribution about the mean direction \( \bar{a} \) of the fiber distribution, \( \bar{a} = a_1 \otimes a_1 \) is the structure tensor associated to the mean direction \( a \) of the fiber distribution, \( \text{i.e., } \psi_f \approx \psi_f^0 + \psi_f^1 \) (1)

\[
\psi_f^1 = \frac{k_1}{2k_2} \exp \left[ k_2 \left( \bar{I}_4 - 1 \right)^2 \right]
\]

\[
\bar{I}_4 = \langle \bar{I}_4 \rangle = H : \bar{\mathbf{C}}, \quad \sigma^2_\alpha = \langle (\bar{I}_4 - \bar{I}_4)^2 \rangle = \mathbb{H} : \bar{\mathbf{C}}
\]
and $H$ and $\mathbb{H}$ define the second and forth order averaged structure tensors, respectively. The model provides a closed form expression of the second Piola-Kirchhoff stress tensor:

$$\bar{\mathcal{S}}_i \simeq \alpha (I^*_4, \sigma^2) H + \beta (I^*_4, \sigma^2) \mathbb{H} : \mathbb{C}$$

which is effective and robust in computational applications.\textsuperscript{14,15,18}

### 2.2. Computational modeling of interweaving variability

The collagen fibril architecture of the stroma is characterized by a regular variation across the thickness, with a marked interweaving in the anterior third and a predominant surface tangent (planar) orientation distribution in the posterior third.\textsuperscript{4,7} The organization of the fibrils can be modelled through a multivariate von Mises distribution, ruling both the in-plane and transverse orientation of the fibrils. Using the spherical angles $[\theta, \Phi] \in [0, \pi], [0, \pi]$ the generic orientation $a$ is:

$$a = \sin \theta \cos \phi \ e_1 + \sin \theta \sin \phi \ e_2 + \cos \theta \ e_3$$

The corresponding PDF, $\rho(a)$, decomposes in out-of-plane term $\rho_\theta(\theta)$ and in-plane term $\rho_\phi(\phi)$ as $\rho(a) = \rho_\theta(\theta) \rho_\phi(\phi)$:

$$\rho_\theta(\theta) = N_\theta \exp[b_\theta \cos 2\theta]$$
$$\rho_\phi(\phi) = N_\phi \exp[b_\phi \cos(\phi - \pi/2)]$$

Fig. 1. Representative example of the multivariate von Mises PDF for three different combinations of the material parameters, $b_\theta$, $b_\phi$. 
The decomposition preserves the simple structure tensor form of the approximated strain energy density. A representative example of multiple combinations is provided in Figure 1.

The formulation allows:

1. to characterize complex spatial PDF by means of only two material parameters, $b_\theta, b_\phi$; and
2. to recover a diagonal form for the averaged structure tensor.

The remarkable computational implication of the approach is that the averaged structure tensors $\mathbf{H}$ and $\mathbb{H}$ depend exclusively on four integral coefficients:

$$
\kappa_\theta = \frac{1}{N_\theta} \int_0^{\pi} \rho_\theta \sin^3 \theta \, d\theta \\
\widehat{\kappa}_\theta = \frac{1}{N_\theta} \int_0^{\pi} \rho_\theta \sin^5 \theta \, d\theta \\
\kappa_\phi = \frac{1}{N_\phi} \int_0^{\pi} \rho_\phi \sin^3 \phi \, d\phi \\
\widehat{\kappa}_\phi = \frac{1}{N_\phi} \int_0^{\pi} \rho_\phi \sin^5 \phi \, d\phi
$$

A representative example of the novel behavior induced by the multivariate PDF is provided in Figure 2 with respect to different values of the concentration parameters $b_\theta, b_\phi$.

### 2.3. Fibril exclusion under compression

A full statistical approach has a great potential to exclude fibrils in compression.$^{15,19}$ By applying the random variable transformation rule, from the PDF of $\theta, \phi$ it is possible to derive the PDFs of $I_4, \rho_{I_4}$ and of $\Psi, \rho_\Psi(\Psi)$. Moreover, by using a principal reference frame,$^{20}$ it is possible to obtain a closed form expression of $\rho_{I_4}(I_4)$ with the
a priori knowledge of the physical integration range. This notable result leads to the correct statistical exclusion of compressed fibers in the mechanical response of the tissue.

3. Conclusion

A material model for fiber reinforced soft materials characterized by stochastic distributions of the fibers is discussed. The approach allows for the description of local smooth variability of the spatial distribution of fibril interweaving, as the one observed across the thickness of the corneal stroma. Moreover, in a principal reference frame description, the knowledge of the portion of compressed fibers is achieved a priori and easily accounted for in numerical calculations. The statistical material model formulation proposed results well suited for multiscale generalization in the context of soft collagenous tissues.21,22

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