

Computational remodeling of the crimped collagen fibril architecture in corneal and scleral tissue

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ABSTRACT

Tissue adaptation and the mechanical condition within biological tissues are complex and mutually dependent phenomena. In this contribution, a computational model is presented to investigate the interaction between collagen fibril architecture and mechanical loading conditions in the cornea and sclera tissue. On the micro-level, collagen fibrils are assumed to crimp into the shape of a cylindrical helix when the tissue is unloaded (Figure 1). The constitutive model for individual fibrils is derived from the nonlinear relation between the 1. Piola-Kirchhoff fiber stress P_{fib} and the fiber stretch λ_{fib} of an extensible helical spring including the fully extension of the spring as a limit case. On the macro-level, the collagen network in eye tissues is represented by means of two families of collagen fibrils. The orientations of individual collagen fibrils \mathbf{e}_0 within each family (fam α with $\alpha = 1, 2$) is considered to be symmetrically dispersed by means of a normalized *von Mises* distribution in the plane spanned by the two vectors $\mathbf{M}_1^{\text{fam}\alpha}$ - $\mathbf{M}_2^{\text{fam}\alpha}$ of the orthonormal frame $\mathbf{M}_j^{\text{fam}\alpha}$, where $\mathbf{M}_1^{\text{fam}\alpha}$ is the mean direction (Figure 2). Following the idea of Gasser et al. [1] a generalized structure tensor is introduced for each fibril family

$$\mathbf{H}_{\text{fam}\alpha} = [(1 - \kappa)\mathbf{M}_1 \otimes \mathbf{M}_1 + \kappa\mathbf{M}_2 \otimes \mathbf{M}_2]_{\text{fam}\alpha} \quad (1)$$

with a single dispersion parameter $\kappa_{\text{fam}\alpha} \in [0; 1/2]$ representing the two-dimensional fibril dispersion in a integral sense. Let the strain energy density of eye tissues be composed of an isotropic part and two

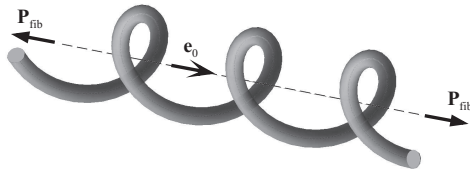


Figure 1: Reference configuration of a single crimped collagen fibril.

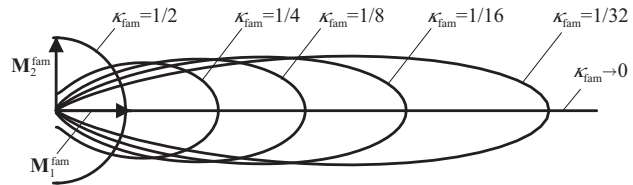


Figure 2: Graphical representation of the distributed fibril orientations \mathbf{e}_0 of one fibril family

anisotropic parts representing the energy contribution of the extrafibrillar matrix and of the two families of crimped collagen fibrils with dispersed orientations

$$W = c(I_{\mathbf{C}} - 3) + \sum_{\alpha=1}^2 \int_1^{\sqrt{\bar{I}_{\mathbf{C}}^{\text{fam}\alpha}}} P_{\text{fib}}(\lambda) d\lambda \quad \text{with } I_{\mathbf{C}} = \text{tr}\mathbf{C}, \bar{I}_{\mathbf{C}}^{\text{fam}\alpha} = \mathbf{H}_{\text{fam}\alpha} : \mathbf{C} \quad (2)$$

under consideration of the incompressibility constraint $\mathbb{I}_{\mathbf{C}} = \det\mathbf{C} = 1$.

The fundamental hypothesis of the proposed remodeling theory is that the orientation of individual collagen fibrils rotate such that after remodeling the collagen network can be again characterized by two generalized structural tensors of the form (1). Accordingly, the biomechanically induced remodeling process can be decomposed into the reorientation of the orthonormal frame $\mathbf{M}_j^{\text{fam}\alpha}$ and into the variation of the dispersion parameter $\kappa_{\text{fam}\alpha}$ of each collagen fibril family. The scalar function used for the definition of the stress based remodeling stimulus is postulated as

$$\Gamma = \begin{cases} \tau_2/\tau_1 & \text{for } \tau_2 \geq 0 \\ 0 & \text{for } \tau_2 < 0. \end{cases} \quad \text{with } \boldsymbol{\tau} = \sum_{i=1}^3 \tau_i \mathbf{n}_i \otimes \mathbf{n}_i \quad \text{and } \tau_1 \geq \tau_2 \geq \tau_3 \quad (3)$$

Herein the spectral decomposition of the Kirchhoff stress tensor $\boldsymbol{\tau}$ is introduced, where τ_i and \mathbf{n}_i are the corresponding eigenvalues and eigenvectors, respectively. The target directions $\mathbf{M}_j^{\text{tar}\alpha}$ of the reorientation process of $\mathbf{M}_j^{\text{fam}\alpha}$ defined at the reference configuration are chosen such that at the current configuration all collagen fibrils tend to reorient into the \mathbf{n}_1 - \mathbf{n}_2 plane, while the mean fibril directions will be located between \mathbf{n}_1 and \mathbf{n}_2 [2]

$$\begin{aligned} \mathbf{M}_1^{\text{tar}1} &= \mathbf{F}_{\otimes}[\cos(\arctan \Gamma)\mathbf{n}_1 + \sin(\arctan \Gamma)\mathbf{n}_2] \\ \mathbf{M}_1^{\text{tar}2} &= \mathbf{F}_{\otimes}[\cos(\arctan \Gamma)\mathbf{n}_1 - \sin(\arctan \Gamma)\mathbf{n}_2] \\ \mathbf{M}_2^{\text{tar}\alpha} &= \mathbf{M}_3^{\text{tar}\alpha} \times \mathbf{M}_1^{\text{tar}\alpha}, \quad \mathbf{M}_3^{\text{tar}\alpha} = \mathbf{n}_3 \mathbf{F} / \|\mathbf{n}_3 \mathbf{F}\| \end{aligned} \quad \text{with } \mathbf{M} = \mathbf{F}_{\otimes}(\mathbf{m}) = \frac{\mathbf{F}^{-1}\mathbf{m}}{\|\mathbf{F}^{-1}\mathbf{m}\|}. \quad (4)$$

The temporal evolution of the frames $\mathbf{M}_j^{\text{fam}\alpha}$ and of the dispersion parameters $\kappa_{\text{fam}\alpha}$ can be expressed by first order rate equations

$$\begin{aligned} \dot{\mathbf{M}}_j^{\text{fam}\alpha} &= \boldsymbol{\omega}_{\text{fam}\alpha} \times \mathbf{M}_j^{\text{fam}\alpha} \quad \text{with } \boldsymbol{\omega}_{\text{fam}\alpha} = \frac{\omega_{\text{tar}\alpha}}{t_{\omega}^*} \mathbf{N}_{\omega}^{\text{tar}\alpha} \\ \dot{\kappa}_{\text{fam}\alpha} &= \frac{1}{t_{\kappa}^*} (\kappa_{\text{tar}\alpha} - \kappa_{\text{fam}\alpha}) \quad \text{with } \kappa_{\text{tar}\alpha} = \Gamma/2, \end{aligned} \quad (5)$$

where $\boldsymbol{\omega}_{\text{tar}\alpha} = \omega_{\text{tar}\alpha} \mathbf{N}_{\omega}^{\text{tar}\alpha}$ is the Rodrigues rotation vector of the rotation tensor $\mathbf{R}^{\text{tar}\alpha} = \mathbf{M}_j^{\text{tar}\alpha} \otimes \mathbf{M}_j^{\text{fam}\alpha}$. In (5) t_{ω}^* and t_{κ}^* can be interpreted as time relaxation parameters of the reorientation process. The remodeling process is introduced into an incompressible finite shell formulation [3], where the incompressibility constraint is enforced through elimination of displacement and strain variables. Finally, the presented approach is applied to a computational human eye model considering the cornea and sclera tissue. After remodeling the predicted fiber morphology correlates well with experimental observations from X-ray scattering data.

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