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A regularised continuum damage model based on the mesoscopic scale for soft tissue

Sergio Blanco *, César Andrés Polindara, Jose María Goicolea

Department of Continuum Mechanics and Structures, School of Civil Engineering, T.U. of Madrid, Profesor Aranguren s/n, 28040 Madrid, Spain

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ABSTRACT

Material properties of soft fibrous tissues are highly conditioned by the hierarchical structure of this kind of composites. Collagen based tissues present, at decreasing length scales, a complex framework of fibres, fibrils, tropocollagen molecules and amino-acids. Understanding the mechanical behaviour at nano-scale level is critical to accurately incorporate this structural information in phenomenological damage models. In this work we derive a relationship between the mechanical and geometrical properties of the fibril constituents and the soft tissue material parameters at macroscopic scale. A Hodge–Petruska two-dimensional model has been used to describe the fibrils as staggered arrays of tropocollagen molecules. After a mechanical characterisation of each of the fibril components, two fibril failures modes have been defined related with two planes of weakness. A phenomenological continuous damage model with regularised softening was presented along with meso-structurally based definitions for its material parameters. Finally, numerical analysis at fibril, fibre and tissue levels are presented to show the capabilities of the model.

1. Introduction

Soft tissues have a hierarchical structure with several scales, from the amino-acids forming the proteins in the atomistic scale to the arterial walls in the continuum scale. The elementary building block of the fibrous reinforcement in soft tissues is collagen. This structural protein consists of tropocollagen (TC) molecules with an aspect ratio close to 200. TC molecules are disposed in staggered arrays forming fibrils which are organised in families of fibres surrounded by an almost incompressible ground matrix (see Baer et al., 1991; Sasaki and Odajima, 1996; Buehler, 2008; Gautieri et al., 2011 among others).

Degradation phenomena in soft tissues have been successfully reproduced through phenomenological damage models (see Balzani et al., 2006; Calvo et al., 2007; Ehret and Itskov, 2009; Peña et al., 2010 among others) although some plasticity-based models have also been presented (see Tanaka and Yamada, 1990; Gasser and Holzapfel, 2002; Itskov and Aksel, 2004). The capabilities and accuracy of these phenomenological models for soft tissues have been improving in the past years. However, less effort has been paid to develop continuum models based on the underlying fracture mechanisms at molecular scale.

The structural mechanisms that control the degradation of soft tissues are related with the behaviour of their fundamental constituents. The study of the relationship between the molecular and intermolecular properties and the tissue behaviour is been actively addressed at present (Buehler, 2006b, 2008; Shoulders and Raines, 2009; Gautieri et al., 2011; Shen et al., 2011 among others). As a consequence, several damage models for soft tissues have been presented derived from the molecular features associated with the tropocollagen molecules. A stochastic, structurally based damage model that considers statistical aspects related to the length distribution of the reinforcing fibres was presented in Rodríguez et al. (2006). A reactive mesoscopic model was presented in Buehler (2008), where tropocollagen molecules are described as a collection of particles interacting according to multibody potentials (see also Buehler, 2006a). Based on these molecular simulations, a multiscale, plasticity based, constitutive model was presented in Tang et al. (2010). Another plasticity based model has been presented in Gasser (2011), where viscoplastic sliding of collagen fibrils is associated with the irreversible degradation of the proteoglycan bridges between them. This model has been applied to the study of the properties of the infrarenal aorta in Martufi and Gasser (2011) and has been enriched with a collagen turnover model in Martufi and Gasser (2012).

In this work we consider the soft tissue as a fibre reinforced composite and the fibre as a fibril reinforced composite. We want

* Corresponding author. Tel.: +34 913365395.
E-mail address: sergio.blanco@upm.es (S. Blanco).

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to physically motivate the irreversible deformation of soft tissues beyond the physiological range of loading. The goal is to explain the damage mechanisms in the fibres using the evolution of their inner structure. In order to do so we assume, as a hypothesis, that inelastic phenomena in the fibre are caused only by degradation processes in the fibrils (Tang et al., 2010). Firstly, we characterise the geometrical and mechanical properties of the fibre components at molecular scale, *i.e.* the tropocollagen molecules in the fibril and the cohesive forces between them. Afterwards, we identify the onset of damage with the development of planes of weakness along the unions between TC molecules. We obtain the macroscale parameters of the fibre from the mesoscale level by numerical homogenisation. In order to pass hierarchically the parameters we have to estimate volume fractions of the fibril within the fibre and of the fibre within the tissue. We have characterised the following macroscopic material parameters of the fibre: the yield strength, the total dissipation energy and the initial size of the elastic domain (that depends on the stored elastic energy density at the onset of damage). Finally we use these structure-derived material parameters to fully characterise a continuum damage model for the fibres. The parameters of this continuum damage model are thus based on the mesoscopic mechanisms within the fibre when irreversible processes take place.

The paper is organised as follows. In Section 2 the methods used in this work are presented: a local damage model for fibrous materials with regularised softening and a mesoscopic-based structural characterisation of the inelastic behaviour of the fibres. Several numerical simulations are included in Section 3, where we perform mechanical analysis at fibril, fibre and tissue levels (all the hierarchical scales we have considered). Finally Section 4 includes the main conclusions of the work.

2. Methods

2.1. A local damage model with regularised softening

We present a material damage model suited for fibrous materials. As stated in Peña et al. (2009), this kind of continuous damage models can reproduce the Mullins' effect only after damage initiation. Two main hypothesis have been considered: the damage processes depend only on the isochoric deformation and each material phase, ground matrix and fibres, damages independently. The model presented here needs only three parameters to characterise the material softening in each phase of the composite: a threshold value that defines the initial size of the elastic domain (usually a limit value of the Cauchy stress or the stretch in the uniaxial homogeneous tension test), a parameter that defines the total amount of internal dissipated energy and a coefficient that affects the rate of softening.

2.1.1. Kinematics

Let $\mathcal{B}_0$ be the reference configuration of the body of interest and $\mathcal{B}_t$ its current configuration. The mapping $\varphi(\boldsymbol{X},t):\mathcal{B}_0\times\mathbb{R}^+\to\mathcal{B}_t$ defines the motion that transforms, at time t, position vectors of the material points $\boldsymbol{X}\in\mathcal{B}_0$ into spatial position vectors $\boldsymbol{x}=\varphi(\boldsymbol{X},t)\in\mathcal{B}_t$. The deformation gradient is defined as $\boldsymbol{F}(\boldsymbol{X},t)=\partial\varphi(\boldsymbol{X},t)/\partial\boldsymbol{X}$, which is multiplicatively decomposed into dilatational and distortional (isochoric) parts (Flory, 1961):

$$\boldsymbol{F}=J^{1/3}\overline{\boldsymbol{F}};\quad \overline{\boldsymbol{F}}=J^{-1/3}\boldsymbol{F}. \tag{1}$$

Eq. (1) allows to obtain the right and left Cauchy–Green deformation tensors, $\boldsymbol{C}$ and $\boldsymbol{b}$, and their corresponding isochoric counterparts:

$$\boldsymbol{C}=\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}=J^{-2/3}\overline{\boldsymbol{F}}^{\mathrm{T}}\overline{\boldsymbol{F}}=J^{-2/3}\overline{\boldsymbol{C}}, \tag{2}$$

$$\boldsymbol{b}=\boldsymbol{F}\boldsymbol{F}^{\mathrm{T}}=J^{-2/3}\overline{\boldsymbol{F}}\overline{\boldsymbol{F}}^{\mathrm{T}}=J^{-2/3}\overline{\boldsymbol{b}}. \tag{3}$$

If we consider n_f families of fibres, the direction of each family at point $\boldsymbol{X}\in\mathcal{B}_0$ is defined by the unit vector $\boldsymbol{a}_{0i}$, with $i=\{1,n_{\mathrm{f}}\}$. The description of these vectors in the current configuration is:

$$\boldsymbol{a}_i=\boldsymbol{F}\,\boldsymbol{a}_{0i};\quad \bar{\boldsymbol{a}}_i=\overline{\boldsymbol{F}}\,\boldsymbol{a}_{0i};\quad \|\boldsymbol{a}_{0i}\|=1, \tag{4}$$

where the macroscopic stretches in the direction of the family of fibres i are defined by $\lambda_i=\|\boldsymbol{a}_i\|>0$ and $\bar{\lambda}_i=\|\bar{\boldsymbol{a}}_i\|>0$. This structure is characterised by a set of generalised structure symmetric tensors (Holzapfel et al., 2000) expressed as:

$$\boldsymbol{H}_i=\boldsymbol{a}_{0i}\otimes\boldsymbol{a}_{0i},\quad i=\{1,n_{\mathrm{fibres}}\}. \tag{5}$$

We assume henceforth our domain of interest has a quasi-incompressible constitutive behaviour and that there are only two families of fibres. The definition of the standard invariants (Spencer, 1971) associated with the distortional deformation

$$\bar{I}_1=\mathrm{tr}\left(\overline{\boldsymbol{C}}\right)=\mathrm{tr}\left(\overline{\boldsymbol{b}}\right)=J^{-2/3}I_1, \tag{6}$$

$$\begin{aligned}\bar{I}_2&=\frac{1}{2}\left[\mathrm{tr}\left(\overline{\boldsymbol{C}}\right)^2-\mathrm{tr}\left(\overline{\boldsymbol{C}}^2\right)\right]\\&=\frac{1}{2}\left[\mathrm{tr}\left(\overline{\boldsymbol{b}}\right)^2-\mathrm{tr}\left(\overline{\boldsymbol{b}}^2\right)\right]=J^{-4/3}I_2,\end{aligned} \tag{7}$$

$$\bar{I}_3=\det\overline{\boldsymbol{C}}=\det\overline{\boldsymbol{b}}=1, \tag{8}$$

$$J=(\det\overline{\boldsymbol{C}})^{1/2}=(\det\overline{\boldsymbol{b}})^{1/2}, \tag{9}$$

$$\bar{I}_4=\overline{\boldsymbol{C}}:\boldsymbol{H}_1=\overline{\boldsymbol{C}}:(\boldsymbol{a}_{01}\otimes\boldsymbol{a}_{01}), \tag{10}$$

$$\bar{I}_6=\overline{\boldsymbol{C}}:\boldsymbol{H}_2=\overline{\boldsymbol{C}}:(\boldsymbol{a}_{02}\otimes\boldsymbol{a}_{02}) \tag{11}$$

allows us to define the following Green–Lagrange strain-like quantities:

$$\bar{E}_1=\overline{\boldsymbol{C}}:\boldsymbol{H}_1-1=\bar{I}_4-1, \tag{12}$$

$$\bar{E}_2=\overline{\boldsymbol{C}}:\boldsymbol{H}_2-1=\bar{I}_6-1, \tag{13}$$

which characterise the strain in the direction of the mean orientations $\boldsymbol{a}_{01}$ and $\boldsymbol{a}_{02}$ (Gasser et al., 2006).

2.1.2. Strain energy function and stress response

Based on the kinematic description of Eq. (1), the strain energy density function can be defined in a decoupled form with a dilatational and an isochoric part. The isochoric contribution can also be decomposed into a part associated with the isotropic behaviour of the ground matrix and a part associated with the anisotropic behaviour of the fibres as:

$$W=U(J)+(1-d_g)\overline{W}_g(\overline{\boldsymbol{C}})+(1-d_{f1})\overline{W}_{f1}(\overline{\boldsymbol{C}},\boldsymbol{H}_1)+(1-d_{f2})\overline{W}_{f2}(\overline{\boldsymbol{C}},\boldsymbol{H}_2), \tag{14}$$

where $\overline{W}_g$, $\overline{W}_{f1}$ and $\overline{W}_{f2}$ represent, respectively, the effective strain energy functions of the hypothetical undamaged materials matrix and fibres. These functions must obey the principle of objectivity and material frame indifference (Holzapfel and Ogden, 2010). Reduction factors $(1-d_g)$, $(1-d_{f1})$ and $(1-d_{f2})$, initially proposed in Kachanov (1958), incorporate the inelastic degradation phenomena taking place separately in the matrix and in each family of fibres, satisfying $0\leqslant d_\alpha\leqslant 1$ for $\alpha=\{g,f1,f2\}$.

Eq. (14) can be expressed in terms of the strain invariants defined in Eqs. (6)–(11) as:

$$W=U(J)+(1-d_g)\overline{W}_g(\bar{I}_1,\bar{I}_2)+(1-d_{f1})\overline{W}_{f1}(\bar{I}_1,\bar{I}_4)+(1-d_{f2})\overline{W}_{f2}(\bar{I}_1,\bar{I}_6). \tag{15}$$

We use the neo-Hookean strain energy function to reproduce the behaviour of the ground matrix and the function proposed in the Holzapfel–Gasser–Ogden model (Holzapfel et al., 2000) to reproduce the behaviour of each family of fibres. Eq. (15) is thus particularised as: