Journal of the mechanical behavior of biomedical materials 68 (2017) 210–215

Contents lists available at ScienceDirect

Journal of the Mechanical Behavior of Biomedical Materials

journal homepage: www.elsevier.com/locate/jmbbm

Development and parameter identification of a visco-hyperelastic model for the periodontal ligament

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ARTICLE INFO

Keywords:
Periodontal ligament
Visco-hyperelastic model
Finite element analysis
Nanoindentation
Parameter identification

ABSTRACT

The present study developed and implemented a new visco-hyperelastic model that is capable of predicting the time-dependent biomechanical behavior of the periodontal ligament. The constitutive model has been implemented into the finite element package ABAQUS by means of a user-defined material subroutine (UMAT). The stress response is decomposed into two constitutive parts in parallel which are a hyperelastic and a time-dependent viscoelastic stress response. In order to identify the model parameters, the indentation equation based on V-W hyperelastic model and the indentation creep model are developed. Then the parameters are determined by fitting them to the corresponding nanoindentation experimental data of the PDL. The nanoindentation experiment was simulated by finite element analysis to validate the visco-hyperelastic model. The simulated results are in good agreement with the experimental data, which demonstrates that the visco-hyperelastic model developed is able to accurately predict the time-dependent mechanical behavior of the PDL.

1. Introduction

The periodontal ligament (PDL) connecting the tooth and the alveolar bone is a connective biological soft tissue. The PDL is primarily responsible for tooth movement for which it does not only govern tooth short-term mobility due to its deformation, but also influences long-term tooth movement (Natali et al., 2008). It is widely accepted that the biomechanical responses in the PDL under orthodontic loads trigger bone remodeling (Kawarizadeh et al., 2003; Natali et al., 2008). Therefore, a detailed understanding of the mechanical properties of the PDL can provide deeper insights into the biomechanical mechanism of tooth movement.

Recently, the mechanical properties of the PDL have been paid considerable attention (Fill et al., 2011, 2012). There are two main ways to investigate the mechanical behavior of the PDL: experimental and computational. There has been a large amount of experimental work surrounding PDL behavior, however, some discrepancies of the results can be found (Fill et al., 2011; Barone et al., 2016). Due to the complex and small scale of the structure, the experimental testing of the mechanical properties for the PDL is still limited. Whereas the process of the experimental testing can be simulated and repeated by the computational methods including finite element analysis (FEA).

FEA requires a practical material model to accurately simulate the biomechanical behavior of the PDL. Most previous studies modeled the PDL as a linear, bilinear, or hyperelastic material (Provatidis, 2001; Limbert et al., 2003; Ziegler et al., 2005; Chang et al., 2014; Huang et al., 2016a). However, experimental evidence shows that the PDL does not only exhibit the instantaneous nonlinear elastic behavior, but also exhibits the time-dependent viscoelastic mechanical property (Dorow et al., 2002; Oskui and Hashemi, 2016; Qian et al., 2009; Sanctuary et al., 2005; Wei et al., 2014). Thus , the coupling of viscoelastic and hyperelastic modeling methods results in a more realistic representation of the PDL.

Natali et al. (2008) developed a visco-hyperelastic constitutive model considering damage of the PDL. Natali et al. (2011) and Oskui et al. (2016) formulated visco-hyperelastic constitutive models coupling a hyperelasticity and stress relaxation by using the internal variables approach. However, FE implementation and validation of the models were not focused on, and the model parameters were determined by means of tensile experimental data of the PDL. Zhurov et al. (2007) proposed a general transversely isotropic visco-hyperelastic model with strain rate based on the thermodynamic constitutive principles, but the identification of the model parameters and FE implementation of the model still need to be addressed due to its stochastic structure.

Mechanical testing of the PDL requires a practical experimental

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http://dx.doi.org/10.1016/j.jmbbm.2017.01.035
Received 26 October 2016; Received in revised form 3 January 2017; Accepted 23 January 2017
Available online 31 January 2017
1751-6161/

model. Due to the complex geometry and micro size of the PDL, it is difficult to adopt the conventional mechanical test methods including the tensile, uniaxial compression, and dynamic shear tests to accurately measure the biomechanical properties of the PDL. However, nanoindentation technology ignoring the geometry of the specimen has been used to characterize the mechanical properties of both soft and hard materials, which provides an effective and promising tool to carry out the present experimental work (Oyen, 2011). Ashrafi and Shariyat (2016) performed nanoindentation experimental testing to identify the parameters of the viscoelastic constitutive models of the PDL by developing indentation creep and relaxation formulas, but the results still need further study.

The objective of the present study is to develop and implement a three-dimensional visco-hyperelastic FE model of the PDL through theoretical modeling in combination with a nanoindentation experiment and its FE simulation. The structural model is formulated within the framework of nonlinear continuum mechanics using the internal variables providing a general description of a material. In order to identify the material parameters and validate the model, nanoindentation experimental tests on the PDL were conducted. The visco-hyperelastic model was used to simulate the nanoindentation experiment through a FE code. Comparison with simulated results and experimental data is performed to validate the model.

2. Material and methods

2.1. Hyperelastic model

For compressible hyperelastic materials, the strain energy function can be decoupled as isochoric and volumetric parts (Limbert et al., 2003)

$$W(\mathbf{C}) = \overline{W}(\bar{I}_1, \bar{I}_2) + W_{\mathrm{vol}}(J) \tag{1}$$

where $\mathbf{C}$ is the right Cauchy-Green deformation tensor, $\bar{I}_1$, $\bar{I}_2$ are the invariants of the isochoric Cauchy-Green deformation tensor $\overline{\mathbf{C}}$, and J is the volume ratio. The incompressible material is characterized by $J = 1$.

An exponential model was proposed by Veronda and Westmann (1970)

$$\overline{W} = C_1(e^{C_2(\bar{I}_1-3)} - 1) + C_3(\bar{I}_2 - 3) \tag{2}$$

where C_1, C_2, and C_3 are model parameters.

The volumetric function is defined as

$$W_{\mathrm{vol}} = \frac{1}{D_1}(J-1)^2 \tag{3}$$

where D_1 is inverse for the bulk modulus.

The second Piola-Kirchhoff stress tensor is derived from Eq. (1)

$$\mathbf{S}^e = 2\frac{\partial W}{\partial \mathbf{C}} = 2\left(\frac{\partial \overline{W}}{\partial \mathbf{C}} + \frac{\partial W_{\mathrm{vol}}}{\partial \mathbf{C}}\right) \tag{4}$$

The Cauchy stress can be calculated using the formula

$$\boldsymbol{\sigma}^e = \frac{1}{J}\mathbf{F}\mathbf{S}^e\mathbf{F}^{\mathrm{T}} \tag{5}$$

Thus, we can obtain

$$\boldsymbol{\sigma}^e = \frac{2}{J}\left[C_1C_2e^{C_2(\bar{I}_1-3)}\left(\overline{\mathbf{B}} - \frac{1}{3}\bar{I}_1\mathbf{1}\right) + C_3\left(\bar{I}_1\overline{\mathbf{B}} - \overline{\mathbf{B}}^2 - \frac{2}{3}\bar{I}_1\mathbf{1}\right)\right] + \frac{2}{D_1}(J-1)\mathbf{1} \tag{6}$$

where $\overline{\mathbf{B}} = \overline{\mathbf{F}\mathbf{F}}^{\mathrm{T}}$ is the isochoric left Cauchy-Green deformation tensor, and $\mathbf{1}$ denotes the second order unit tensor.

For incompressible materials, the Cauchy stress is given as

$$\boldsymbol{\sigma}^e = 2C_1C_2e^{C_2(I_1-3)}\mathbf{B} + 2C_3(I_1\mathbf{B} - \mathbf{B}^2) + p\mathbf{1} \tag{7}$$

where p is the hydrostatic pressure.

2.2. Visco-hyperelastic model

The general constitutive model equation of a nonlinear visco-hyperelastic material was stated as (Pawlikowski, 2013)

$$\mathbf{S}(t) = g_\infty\mathbf{S}^e + \sum_{i=1}^{N}\int_0^t g_i\cdot e^{-t/\tau_i}\frac{\partial \mathbf{S}^e(s)}{\partial s}\mathrm{d}s \tag{8}$$

where g_i are the relative shear relaxation modulus of term i, and $g_\infty + \sum_{i=1}^{N} g_i = 1$. The time-dependent relaxation function $g(t)$ can be defined by means of the Prony series

$$g(t) = g_\infty + \sum_{i=1}^{N} g_i\cdot e^{-t/\tau_i} \tag{9}$$

where τ_i and N are relaxation times and number of them, respectively.

In Eq. (8), the internal algorithmic history variables are given as

$$\mathbf{H}_i(t) = \int_0^t g_i\cdot e^{-t/\tau_i}\frac{\partial \mathbf{S}^e(s)}{\partial s}\mathrm{d}s \tag{10}$$

For the time interval $[t_n, t_{n+1}]$, the time step is defined as $\Delta t = t_{n+1} - t_n$, and using the integral algorithm presented by Kaliske (2000), Eqs. (8) and (10) can be written in the updated form, respectively

$$\mathbf{S}_{n+1} = g_\infty\mathbf{S}^e_{n+1} + \sum_{i=1}^{N}\mathbf{H}_{i,n+1} \tag{11}$$

and

$$\mathbf{H}_{i,n+1} = e^{-t/\tau_i}\mathbf{H}_{i,n} + g_i\frac{1-e^{-t/\tau_i}}{\Delta t/\tau_i}(\mathbf{S}^e_{n+1} - \mathbf{S}^e_n) \tag{12}$$

The Cauchy stress for visco-hyperelastic model is given by

$$\boldsymbol{\sigma}_{n+1} = \frac{1}{J_{n+1}}g_\infty\mathbf{F}_{n+1}\mathbf{S}^e_{n+1}\mathbf{F}^{\mathrm{T}}_{n+1} + \frac{1}{J_{n+1}}\sum_{i=1}^{N}\mathbf{F}_{n+1}\mathbf{H}_{i,n+1}\mathbf{F}^{\mathrm{T}}_{n+1} \tag{13}$$

Jacobian matrix in the material description is obtained as

$$\mathbb{C}_{n+1} = \left(g_\infty + \sum_{i=1}^{N} g_i\frac{1-e^{-t/\tau_i}}{\Delta t/\tau_i}\right)\mathbb{C}^e_{n+1} \tag{14}$$

with

$$\mathbb{C}^e_{n+1} = 2\frac{\partial \mathbf{S}^e_{n+1}}{\partial \mathbf{C}_{n+1}} \tag{15}$$

Use the push-forward operator

$$\mathbb{C}^J_{n+1} = \frac{1}{J}\mathbf{F}_{n+1}\mathbf{F}_{n+1}\mathbb{C}_{n+1}\mathbf{F}^{\mathrm{T}}_{n+1}\mathbf{F}^{\mathrm{T}}_{n+1} \tag{16}$$

In ABAQUS, the Jaumann rate is provided for a suitable objective rate, so the Jacobian matrix can be written in the form

$$\mathbb{C}^{\sigma J}_{n+1} = \mathbb{C}^J_{n+1} + \mathbb{Q}_{n+1} \tag{17}$$

with

$$\mathbb{Q}_{n+1} = \frac{1}{2}(\delta_{ik}\sigma_{jl} + \sigma_{ik}\delta_{jl} + \delta_{il}\sigma_{jk} + \sigma_{il}\delta_{jk})_{n+1}\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k\otimes\mathbf{e}_l \tag{18}$$

where δ_{ij} is the Kronecker delta.

The visco-hyperelastic model was implemented into the general purpose FE software ABAQUS through developing a user-defined material subroutine (UMAT).

2.3. Experiments

In order to identify the parameters of the visco-hyperelastic model and validate the model, the experimental data in the present study is same as our previous work in which the experiment was only used to