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On a mathematical model of a human root dentin

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Summary *Objective*: On the basis of recent experimental data, a new mathematical model that predicts creep in human root dentin has been developed.

Method: The chosen constitutive model comprises fractional derivatives of stress and strain and the restrictions on the coefficients that follow from the Clausius–Duhem inequality.

Results: The four constants describing mechanical properties of the human dentin at constant temperature are calculated from a highly non-linear system involving Mittag–Leffler-type functions. Special attention is paid to thermodynamical restrictions that should be observed in determining parameters of the model from experimental results.

Significance: The proposed model allows us to predict behavior of a human dentin in different load situations. Also it could be used for describing mechanical properties of dentin that are important in the development of 'dentin-like' restorative materials.

Introduction

Determination of mechanical properties of human dentin has an importance from both pragmatic and theoretical point of view. In the case where dentin is modeled as an elastic body (homogeneous, isotropic), two constants (modulus of elasticity and Poisson's ratio, for example) completely determine mechanical behavior at constant temperature. Taking into account the structure of human dentin, that is, its highly oriented tubular structure with a varying percentage area of tubules in the total area of the dentin,[1] more complicated mechanical models must be used.

Dentin is vital hydrated composite material composed of organic and inorganic phase. The following facts concerning human dentin are of importance:

1. The composition of human dentin is approximately 70% inorganic, 20% organic material and 10% water by weight.
2. The inorganic phase of dentin is mainly apatite crystallites similar in size to those seen in bone and cementum, and an organic phase consisting primarily of type 1 collagen.
3. The microstructural characteristic of human dentin is the arrangement of dentinal tubules (the number of tubules, ranges from (19–45)1000/mm^2 with the mean diameter (0.8–2.5) μm), small canals that extend through the entire dentin thickness, from the dentino-enamel or dentino-cemental junction to the pulp.

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The course of the dentinal tubules is radial and slightly S-shaped in the crown but more straight at incisal portions and in the root. Dentinal tubules are filled with odontoblastic processes and dentinal fluid. Each dentinal tubule is lined with a layer of peritubular dentin, which is much more mineralized than the surrounding intertubular dentin. Pashley et al.[1] reported that number of tubules and peritubular dentin area decrease with distance from the pulp and the intertubular area increases with distance from the pulp.

4. The composition and microstructure of dentin is well-known but there are fewer studies about the relationship between the structure and mechanical properties of human dentin.

Our aim in this work was to propose a viscoelastic fractional-derivative model of human dentin. Fractional-derivative models have been used with great success to describe stress relaxation and creep phenomena for different materials. Here we shall show that the results of Ref. 2 can be nicely described by a fractional-derivative viscoelastic model. The mechanical properties of human dentin are important to the development of 'tooth-like' or 'dentin-like' restorative materials.

The model

It is known that Hooke's law, describing strain (relative elongation) ε and stress (force per unit area of the body in the undeformed state), also called Piola–Kirchhoff stress[3] states

$$\sigma = \bar{E}\varepsilon, \tag{1}$$

where the constant $\bar{E} > 0$ is called the modulus of elasticity. The standard linear viscoelastic body has a constitutive relation (stress–strain relation) in the form

$$\sigma + \tau_\sigma \sigma^{(1)} = \bar{E}\varepsilon + \bar{E}\tau_\varepsilon \varepsilon^{(1)}, \tag{2}$$

where σ and ε denote the stress and strain at time t, respectively, $(\cdot)^{(1)} = \mathrm{d}(\cdot)/\mathrm{d}t$ denotes the first derivative with respect to time, and τ_σ, $\bar{E}$ and τ_ε are constants called stress relaxation time, modulus of elasticity and strain relaxation time, respectively. The second law of thermodynamics, together with the stability conditions implies that in Eq. (1) the following restrictions on the constants must be satisfied[8,9]

$$\bar{E} > 0, \qquad \tau_\sigma > 0, \quad \tau_\varepsilon > \tau_\sigma. \tag{3}$$

To describe the specific class of viscoelastic materials, equations of type (2) have been generalized by replacing the first derivative that appears in Eq. (2) with the fractional derivatives. Thus, if we introduce α—the derivative, $0 < \alpha < 1$, of a function $f(t)$ in the Riemann–Liouville form[4,5,10]

$$\frac{\mathrm{d}^\alpha}{\mathrm{d}t^\alpha} f(t) = f^{(\alpha)} \equiv \frac{\mathrm{d}}{\mathrm{d}t} \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f(\tau)\mathrm{d}\tau}{(t-\tau)^\alpha},$$

where Γ is the Euler gamma function, then the fractional derivative type generalization of Eq. (2) was taken in the form, see Ref. 6, for example

$$\sigma + a\sigma^{(\alpha)} = E\varepsilon + Eb\varepsilon^{(\alpha)}, \tag{4}$$

where $0 < \alpha < 1$ and a, b and E are constants. The dimension of a and b is time to the power of α.

By invoking the second law of thermodynamics, the following restrictions on the constants α, a, b and E are obtained[6,7]

$$E > 0, \qquad b \geq a > 0. \tag{5}$$

We shall use constitutive equation (5) to study stress relaxation and creep.

By applying the Laplace transform $L(f)(z) = \int_0^\infty e^{itz} f(t)\mathrm{d}t = \bar{f}(z)$ to Eq. (4) we obtain

$$\bar{\sigma}(1 + az^\alpha) = E\bar{\varepsilon}(1 + bz^\alpha), \tag{6}$$

where we used the fact that

$$L[y^{(\alpha)}] = z^\alpha \bar{f}(z) - \left(\frac{1}{\Gamma(1-\alpha)} \int_0^t y(\tau)(t-\tau)^{-\alpha}\mathrm{d}\tau\right)_{t=0}.$$

The term

$$\left(\left(\frac{1}{\Gamma(1-\alpha)} \int_0^t y(\tau)(t-\tau)^{-\alpha}\mathrm{d}\tau\right)\right)_{t=0}$$

vanishes if $y(t)$ is bounded for $t \to +0$. Eq. (6) was solved for $\bar{\varepsilon}$ or for $\bar{\sigma}$ to obtain

$$\bar{\varepsilon} = \frac{\bar{\sigma}}{E}\left[1 - \left(1 - \frac{a}{b}\right)\frac{z^\alpha}{z^\alpha + \frac{1}{b}}\right], \tag{7}$$

or

$$\bar{\sigma} = E\bar{\varepsilon}\left[1 + \left(\frac{b}{a} - 1\right)\frac{z^\alpha}{z^\alpha + \frac{1}{a}}\right]. \tag{8}$$

The inversion of Eqs. (7) and (8) could be easily obtained, (see, for example, Ref. 11, p. 292)

$$\varepsilon(t) = \frac{\sigma(t)}{E} - \frac{1}{E}\left(1 - \frac{a}{b}\right)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \sigma(t-\tau)e_\alpha\left(\tau; \frac{1}{b}\right)\mathrm{d}\tau, \tag{9}$$

where $e(t;\lambda)$ is the Mittag-Leffler-type function, defined as[12]

$$e_\alpha(t;\lambda) = E_\alpha(-\lambda t^\alpha), \tag{10}$$

with $E_\alpha(t)$ being the Mittag-Leffler function ($\alpha > 0$),

$$E_\alpha(t) = \begin{cases} \sum_{n=0}^{\infty} \frac{t^n}{\Gamma(\alpha n+1)}, & \text{for small } t \\ -\sum_{k=1}^{\infty} \frac{t^{-k}}{\Gamma(1-\alpha k)}, & \text{for large } t \end{cases} \tag{11}$$

Similarly from Eq. (8) we obtain

$$\sigma(t) = E\left[\varepsilon(t) + \left(\frac{b}{a}-1\right)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \varepsilon(t-\tau)e_\alpha\left(\tau;\frac{1}{a}\right)\mathrm{d}\tau\right]. \tag{12}$$

With this preparation completed, we apply Eqs. (9) and (12) to creep and stress relaxation tests, respectively.

Creep test

Suppose that

$$\sigma(t) = \begin{cases} 0, & t \le 0 \\ \sigma_0, & t > 0 \end{cases}. \tag{13}$$

Then, from Eq. (9) we obtain

$$\varepsilon(t) = \frac{\sigma_0}{E}\left[1 - \left(1-\frac{a}{b}\right)e_\alpha\left(t;\frac{1}{b}\right)\right]. \tag{14}$$

Stress relaxation test

Similarly suppose that

$$\varepsilon(t) = \begin{cases} 0, & t \le 0 \\ \varepsilon_0, & t > 0 \end{cases}. \tag{15}$$

then Eq. (12) leads to

$$\frac{\sigma(t)}{E\varepsilon_0} = 1 + \left(\frac{b}{a}-1\right)e_\alpha\left(t;\frac{1}{a}\right). \tag{16}$$

Results of application to the measurements of human root dentin

We applied the model presented in Section 2 to the experimental results presented in Ref. 2. Namely, our model depends on four parameters α, a, b and E. Four points were chosen from the stress relaxation curve presented in Fig. 6 of Ref. 2 and then Eq. (16) was forced to pass through those points. In doing so, we used Newton's method. Then we used the least squares method to improve the agreement between the model and the experimental results. For the case presented in Fig. 6 of Ref. 2, the suggested procedure yields

$$\alpha = 0.136,\ a = 0.525,\ b = 0.778,\ E\varepsilon_0 = 616.287. \tag{17}$$

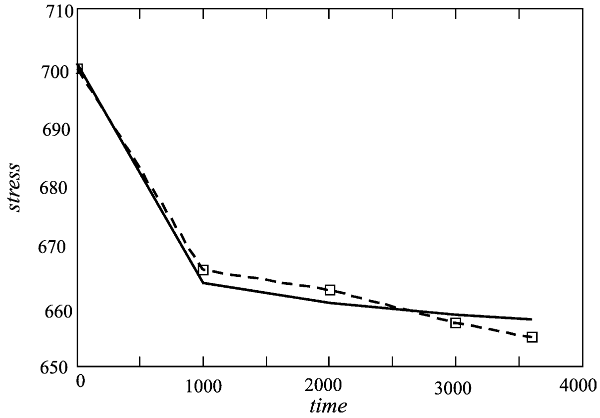

Figure 1 Agreement between the stress relaxation curves for the sample loaded to 700 NT (dashed line) of Ref. 2 and the fractional models (16) and (17).

In Fig. 1, the agreement between the experimental results and the model (16) with (17) can be seen.

We note that the maximal relative error is less then 3%. This is an important property of this model: it is simple, it has a small number of parameters (E, a, $b$and α) and it is able to predict behavior of the material with significant accuracy.

In Fig. 2, we show the stress relaxation curve predicted by the fractional model for large values of time.

Two remarks can be made here. First, it should be noted that the constants (17) could be used for different types of loading,[13,14] such as impact and cyclic loading. Also, it should be noted that

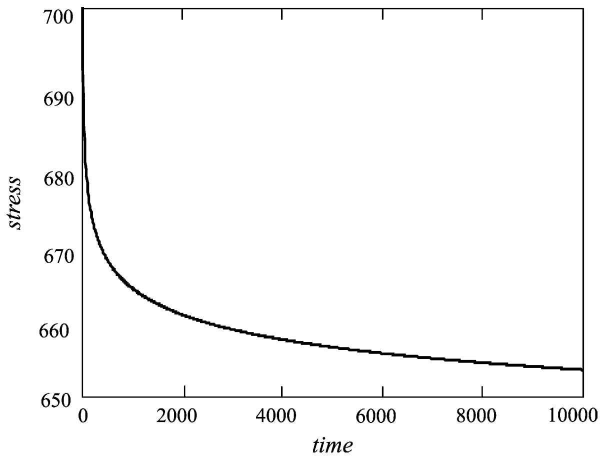

Figure 2 Prediction of stress relaxation in dentin.

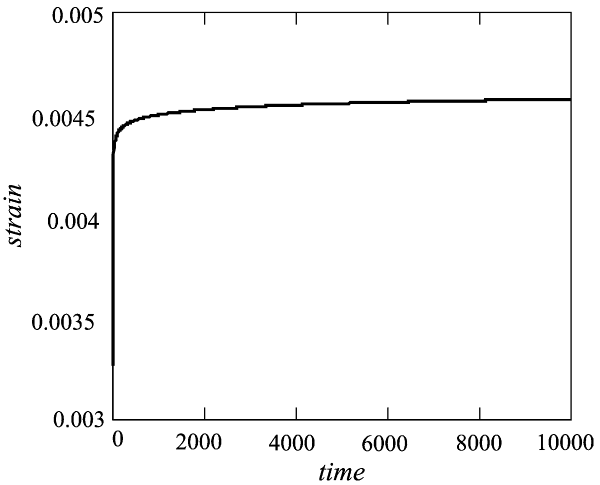

Fig. 3 Prediction of creep in dentin.

the constants α, a, b and E could be estimated for different values of temperature and then used for predictions of dentin behavior in real clinical situations. Both remarks are important for restorative dentistry, since it is expected that dentin-like materials, chosen for restoration, will give better results than others.

Finally as another test of this model we predict creep of dentin, see Fig. 3. Namely, we put Eq. (17) and $\sigma_0 = 300$ N in Eq. (14) and obtain the creep curve very close to the experimental curve presented in Fig. 3 of Ref. 2.

Conclusions

In this work, we proposed a fractional-derivative viscoelastic model (6) for describing mechanical properties of a human root dentin. When applied to creep and stress relaxation tests, this model lead to the expressions (16) and (17) which it was expected would accurately match the experimental results.

The experimental results presented in Ref. 2 were used to determine the four constants in the proposed model. We found good agreement between the experimental results and the theoretical prediction.

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