PHYSICAL REVIEW E **79**, 030903(R) (2009)

Probabilistic model of ligaments and tendons: Quasistatic linear stretching

M. Bontempi*
Biomechanics Laboratory, Istituti Ortopedici Rizzoli, via di Barbiano 1/10, 40136 Bologna, Italy
(Received 25 September 2008; revised manuscript received 11 February 2009; published 12 March 2009)

Ligaments and tendons have a significant role in the musculoskeletal system and are frequently subjected to injury. This study presents a model of collagen fibers, based on the study of a statistical distribution of fibers when they are subjected to quasistatic linear stretching. With respect to other methodologies, this model is able to describe the behavior of the bundle using less *ad hoc* hypotheses and is able to describe all the quasistatic stretch-load responses of the bundle, including the yield and failure regions described in the literature. It has two other important results: the first is that it is able to correlate the mechanical behavior of the bundle with its internal structure, and it suggests a methodology to deduce the fibers population distribution directly from the tensile-test data. The second is that it can follow fibers' structure evolution during the stretching and it is possible to study the internal adaptation of fibers in physiological and pathological conditions.

DOI: 10.1103/PhysRevE.79.030903 PACS number(s): 87.85.Tu, 46.70.Hg, 62.20.M−, 81.40.Lm

Ligament and tendon injury can be very serious both for nonathletes and athletes, and when it happens, it is fundamental that physicians do their best to ensure a correct repair of the injury. The literature presents many clinical articles concerning hypotheses and proposals about techniques useful to repair ligaments correctly. Response to this demand can be found through mechanical measurements and the development of a models to cover a wider range of applications, from specific to general ones. The first to describe tendon behavior was Abrahams in 1967 [1], who also described the properties of tendon samples, in nonphysiological conditions. In 1991, Blankevoort *et al.* [2] published a paper describing how ligament fibers were recruited during knee flexion and they found that the tension on the ligament depends on the recruited fibers and their length (or strain). Between 1996 and 1997, Mommersteeg, Blankevoort, and coworkers [3–5] proposed a model of the knee where they used nonlinear dynamics to model ligaments and described ligaments as being made of different bundles, each one with its different mechanical properties and functions. These articles were followed by others that described models based on continuum mechanics. Pioneers in this field are Fung [6] and Woo [7,8] who used constitutive equations to model the collagen fibers and predict the stress-strain behavior. These models work well during fiber recruitment and linear elastic deformation phases [9,10] but nothing is said about bundle failure. Although these models are effective at describing the force-stretch behavior of bundles, *ad hoc* hypotheses need to be made about the equations to insert into the models, and the result could vary greatly depending on the change of equations. These types of models can describe the viscoelastic behavior of collagen bundles and can be solved numerically using finite element method, but, as reported by Donahue *et al.* [11], it is important to know the accurate three-dimensional geometric structure of the joint, how the joint components interact each others, and how to make meshes to describe the joint structures (bones, ligaments, tendons). Another approach, that can be used to model a collagen bundle, is to look at collagen fibers as a statistic population and correlate the single fiber dynamics through the population [12–14]. This is the core of the model presented here. It is based on the assumption that Nature creates ligaments and tendons with a specific structure according to the specific function. For this reason this model wants to avoid, as much as possible, *a priori* hypotheses on the internal structure, because it wants to suggest methods to create specific models for specific bundles. Because this is a very challenging goal, the most simplified case is presented here, but other features are going to be added, such as continuum mechanics formalism, geometrical structure, viscoelastic behavior and temperature dependence [15]. This is the first step of a project for the development of a complete model of ligaments and tendons, and its final goal is the description of the thermodynamics of collagen bundles.

Collagen fibers have a very complex anatomical structure, both concerning their molecular composition and their structural organization. As reported in the literature [16], the bundle is described by a hierarchical structure which was schematically described by Kastelic *et al.* [17]: *collagen fibers* are arranged together in *microfibrils* and these are grouped in a super structure called *subfibrils*, and so on to *fibrils, fascicles*, and, at the end, *tendons* or *ligaments* (*bundles*), as shown in Fig. 1. The model here described analyzes what happens to a collagen bundle when it is quasistatically stretched and, for this reason, the spatial distribution of fibers can be ignored. Each collagen fiber is considered as a one-dimensional string characterized by a rest length (x_r), and a maximal length (x_b), after which it fails

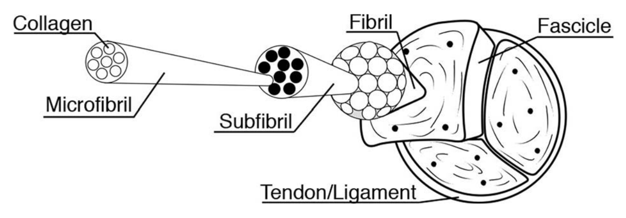

FIG. 1. Representation of the hierarchical structure of tendons and ligaments.

*m.bontempi@biomec.ior.it

and is supposed to have a force response to stretching $f(x)$, so that $f(x)\neq 0$ if $x\in[x_r,x_b[$ and $f(x)=0$ otherwise.

First step—recruitment. A collagen bundle is made by a population of collagen fibrous structures. As described by Kastelic and co-workers in 1980 [18,19], as the bundle stretch increases, the fibers are recruited and the bundle stiffness begins to increase (toe phase). After all fibers have been recruited, they enter into the elastic phase. The fiber recruitment mechanism was modeled by Woo [7,20] and Fung [6] and considered the stress-strain nonlinear behavior of the bundle. A simplified version of the Woo and Fung approach is used as the first step of this model and considers a population of linear elastic fibers one-dimensionally stretched. Because of the presence of the rest length, the model takes into account only the stretch length ($L\geqslant 0$). In the phase of recruitment, the fiber population can be characterized by the numbers of fibers (N_0) distributed according to a certain probability density of the rest lengths, with a mean and standard deviation of the population: $r(x;\bar{x}_r,\sigma_r)$. In this case, the fibers recruited between x and $x+dx$ have a length $L-x$, so the equation of force is

$$F(L)=N_0\int_{-\infty}^{L} r(x;\bar{x}_r,\sigma_r)f(L-x)dx. \tag{1}$$

The "$-\infty$" at the lower bound of the integral takes into account the *pretension*, i.e., the bundle could have a physiological initial tension, so it can have a nonzero force when $L=0$.

Second step—failure: The next step is to model what happens when the stretch increases too much and fibers begin to fail. Collagen fibers have their own failure length and, as above, it is possible to consider the distribution of the failure lengths: $b(x;\bar{x}_b,\sigma_b)$. Because the force depends on the fibers' integrity, Eq. (1) is changed to take into account the probability that fibers are intact during stretching:

$$F(L)=N_0\int_{-\infty}^{L} r(x;\bar{x}_r,\sigma_r)f(L-x)[1-B(L-x)]dx, \tag{2}$$

where $B(L-x)=\int_{-\infty}^{L-x}b(\lambda;\bar{x}_b,\sigma_b)d\lambda$ is the probability of failure after a fiber stretch of $L-x$.

It is now necessary to study the properties of Eq. (2) to see if it is able to describe bundle behavior. Equation (2) gives the tensile relation between stretch and bundle load and correlates them with the internal organization of fibers. In fact, it is a function not only of the stretch length, but also of the statistical parameters of the population: $F(L)=F(L;N_0,\bar{x}_r,\sigma_r;\bar{x}_b,\sigma_b)$. Looking at Eq. (2) it can be seen that while the fiber's integrity probability acts only in the yield and failure regions, the recruitment function works on all the aspects and it is a very important part in the bundle behavior. It is also clear which is the main role of each parameter in the curve: $\bar{x}_r$ acts on the pretension, σ_r determines the toe region length and the failure slope, $\bar{x}_b$ affects the length of the linear region and σ_r determines the yield region length and the failure slope. Other crucial "parameters" are the forms of the probability functions and the fiber's force function which are discussed later. The dependences of the model can be used to fit experimental data and the fitting parameters can be useful to evaluate fiber properties. It is also possible to make a comparison of different bundles types. Concerning the probability properties, it is evident that during fiber stretching there is an increase in the number of recruited fibers, with a consequent increase in force (toe region). When all the fibers are recruited $[\int_{-\infty}^{L}r(x)dx\approx 1]$ and most of them are intact $[1-B(L-x)\approx 1]$, the force becomes linear with the stretch (linear region) and the slope is determined by function $f(L-x)$. Because of the decrease in intact probability with stretching, when the force becomes big enough, the number of intact fibers begins to decrease and the bundle force decreases in slope and stiffness (yield region) until the force reaches a maximum. After the maximal load, the fiber integrity breaks down, because of the creation of stress concentration regions, and the force rapidly decreases to zero (failure region) and in this case this model fails its description with respect to the real bundle, because it does not contain the stress concentration effects. Changes in the fiber population in the load regions, during the tensile test, can be analyzed by evaluating the fiber density distribution:

$$n(x)=N_0 r(x)[1-B(L-x)] \tag{3}$$

with $x\in[0,L]$. The population analysis is important to correlate bundle behavior to changes inside its structure. This could be used to study a partially injured population in the bundle and compare it with the normal bundle, to study how fiber integrity is connected to the bundle laxity, which is crucial for joint stability [2,3,7,15,21]. The derivative of Eq. (2), with respect to the stretch, gives information about the linear slope and about the position of the maximal force of the bundle (for conciseness from now on the substitution $y=L-x$ is made in all the following equations):

$$\frac{dF}{dL}=N_0\int_{-\infty}^{L} r(x)\{f_L'(y)[1-B(y)]-f(y)b(y)\}dx, \tag{4}$$

where $f_L'(y)=\frac{\partial f}{\partial L}(y)$. The maximal force stretch can be found by resolving the equation $\frac{dF}{dL}=0$. The second derivative gives more fundamental information:

$$\frac{d^2F}{dL^2}=N_0 f_L'(0)r(L)-N_0\int_{-\infty}^{L} r(x)\times\left\{f_L''(y)[1-B(y)]-2f_L'(y)b(y)+f(y)\frac{db(y)}{dy}\right\}dx \tag{5}$$

with $f_L''(y)=\frac{\partial^2 f}{\partial L^2}(y)$. If the following conditions are valid in toe and linear regions:

$$\begin{cases} f_L'(0)=C\neq 0 \\ f_L''(y)\ll 1 \quad \forall\, y\in[0,L] \end{cases}, \tag{6}$$

the integral in Eq. (5) is negligible and the equation can be approximated as

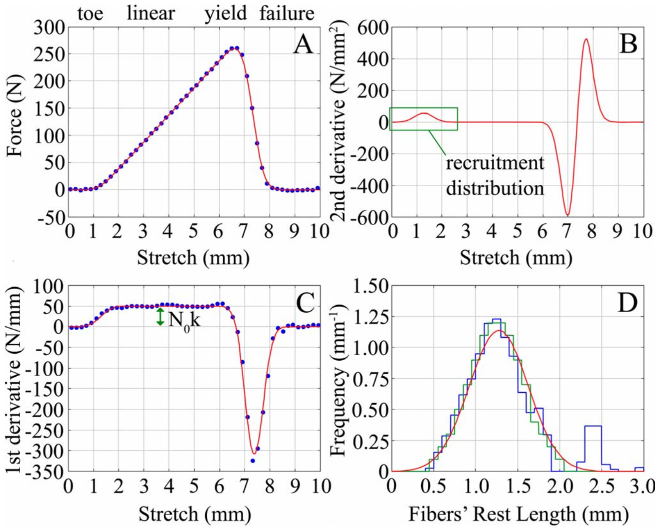

FIG. 2. (Color online) Tensile test data fitted using Eq. (8). Plots (A) and (B) show experimental data and the model fitting and their first derivative. Plot (C) shows the second derivative of data and highlights the results of Eq. (7) and plot (D) shows the comparison of the model distribution (red line) with the data generator (green histogram) and the second numerical derivative of the data set (blue histogram).

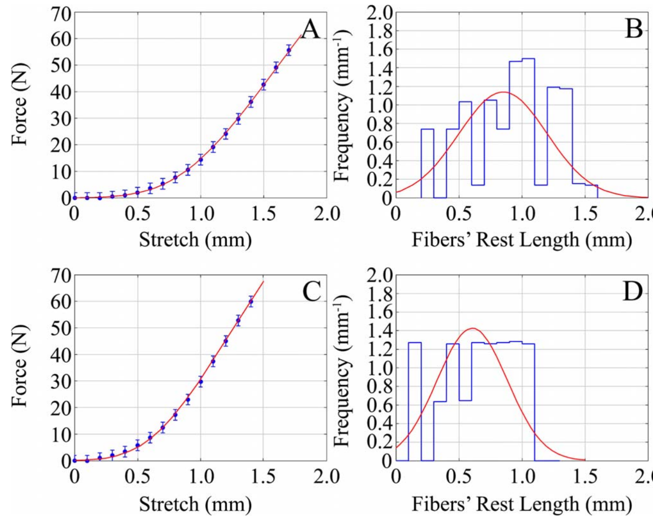

FIG. 3. (Color online) Tensile data fitting of Gracilis (A) and Semitendinous (C) tendons using Eq. (8). Panels (B) and (D) show the respective histograms of the recruitment fiber length distribution and the gauss distribution used to fit tensile data with Eq. (9).

$$\frac{d^2F}{dL^2} \simeq [N_0C]r(L) \tag{7}$$

and it is possible to have a direct evaluation of the recruitment distribution of the fiber population inside the bundle. This has a tremendous implication because it frees the model from *a priori* hypotheses about the fiber length distribution and also suggests an experimental method to extrapolate the real form of $r(x;\bar{x}_r,\sigma_r)$ specific for each type of bundle. It is therefore possible to make an accurate tensile test in the toe and linear regions, and then, evaluate numerically the second derivative, to determine the statistical properties and the typology of the recruitment distribution, and create a bundle database useful to make *ad hoc* models.

The correctness of the model was first tested fitting data generated by a Monte Carlo simulation. Eppel *et al.* [22] measured the force-displacement relation of a single collagen fibril and they found a quasilinear behavior. With this result, the model was tested using a linear form of the single fiber force $f(y)=ky$ where k is the fiber elastic constant, and Eq. (2) can be written as

$$F(L) = N_0k\int_{-\infty}^{L} r(x)y[1-B(y)]dx. \tag{8}$$

In this case the conditions (6) are valid in fact $f'_L(0)=k$ and $f''_L(y)\equiv 0\,\forall\, y$ and it is possible to have an evaluation of the fibers population using the approximation in Eq. (7):

$$\frac{d^2F}{dL^2} \simeq [N_0k]r(L). \tag{9}$$

Figure 2 shows the results of the simulation of 10^6 linear fibers with a force response of $f(x)=k(x-x_r)\,\forall\, x\in[x_r,x_b[$ and $f(x)=0$ otherwise. All the simulation's parameters were randomly generated and both the rest length of each fiber (x_r) and the break length (x_b) were Gaussian distributed, including the *extra* noise added to the total fiber's force. The data set was fitted according to the model in Eq. (8) and the derivatives are fitted applying a denoise filter. As can be seen in Fig. 2(a) the model is able to describe the experimental data with an optimal approximation (including the failure region because the data set generator does not take into account the stress concentration effects) and it is able to infer the recruitment rest length distribution according to Eq. (7) [Fig. 2(d)]. The recruitment population distribution was also tested with data from [15] and results are shown in Fig. 3. The differences between Figs. 3(b) and 3(d) show that the fiber length population could be very variable according to the specific type and function of the bundle. In this case, the number of points is too poor to give an accurate description of the population using the approximated equation (7), but it is evident that the Gracilis tendon fibers have a Gaussian-type distribution [Fig. 3(b)], whereas in the Semitendinous tendon the distribution is not Gaussian, but seems to be uniform after a certain length [Fig. 3(d)]. This difference is too small to be detected in the tensile data fitting [Figs. 3(a) and 3(c)]. The extraction of the recruitment distribution is important information that can be obtained directly from tensile tests and can be used to characterize the fibers microscopically and make a theoretical model of the bundle properties. During the data fitting tests, it was observed that the model parameters are sensitive to changes of the order of 0.01 mm and this must be taken into account as a resolution suggestion for the experimental evaluation of the recruitment population derived from Eqs. (4) and (5).

The model analyzes the easiest aspect of the collagen bundle behavior (i.e., quasistatic, linear stretching), but it shows its ability to describe and explain the results of the literature correctly and gives interesting descriptions about the internal organization of the bundle. The originality and the advantage of the approach used here is that it can describe all the behaviors presented in the literature, including the yield and part of the failure phases, thus avoiding many *ad hoc* hypotheses, and it can neglect the accuracy of the geometry description. Despite other probabilistic models this does not need the *a priori* knowledge of the probability functions and it suggests a methodology to extract these information from the experimental data, opening the opportunity to make specific models according to the bundle characteristics, as expected. It could have several applications in biomechanics to correlate ligament and tendon functions to anatomical parameters and to understand better how macroscopic behavior is correlated to the microscopic structure of the bundle, and evaluations can be made about the physiological and pathological structure and behavior of the bundle. The latter could be very beneficial in ligament reconstruction and prosthesis implantation with a complete theory. Moreover, a comparison of bundle properties could be used to evaluate which bundle is suitable to reconstruct an injured ligament when many different tendons could be used [23]. Another important clinical application in ligament reconstruction is the evaluation of the ligament pretension and graft tension, which are crucial for the outcome of the intervention [24,25]. This model is the first step in the development of a complete description of ligaments and tendons. The next step in the model's development road map is the integration of the results obtained here with the continuum mechanics and the theory of elasticity.

[1] M. Abrahams, Med. Biol. Eng. **5**, 433 (1967).
[2] L. Blankevoort, R. Huiskes, and A. de Lange, J. Biomech. Eng. **113**, 94 (1991).
[3] T. J. A. Mommersteeg, L. Blankevoort, R. Huiskes, J. G. Kooloos, and J. M. G. Kauert, J. Biomech. **29**, 151 (1996).
[4] L. Blankevoort and R. Huiskes, J. Biomech. **29**, 955 (1996).
[5] T. J. A. Mommersteeg, R. Huiskes, L. Blankevoort, J. G. Kooloos, and J. M. G. Kauert, J. Biomech. **30**, 139 (1997).
[6] Y. C. Fung, *Biomechanics: Mechanical Properties of Living Tissues* (Springer, New York, 1993).
[7] S. L.-Y. Woo, S. D. Abramowitch, R. Kilger, and R. Liang, J. Biomech. **39**, 1 (2006).
[8] S. L.-Y. Woo, M. B. Fisher, and A. J. Feola, Mol. Cell. Biomech. **5**, 49 (2008).
[9] Y. Lanir, J. Biomech. **16**, 1 (1983).
[10] Y. Lanir, Biophys. J. **24**, 541 (1978).
[11] T. L. Haut Donahue, M. L. Hull, M. M. Rashid, and C. R. Jacobs, J. Biomech. Eng. **124**, 273 (2002).
[12] A. J. Rapoff, D. M. Heisey, and R. Vanderby, Jr., J. Biomech. **32**, 189 (1999).
[13] C. Hurschler, P. P. Provenzano, and R. Vanderby, Jr., J. Biomech. Eng. **125**, 415 (2003).
[14] C. Hurschler, B. Loitz-Ramage, and R. Vanderby, Jr., J. Biomech. Eng. **119**, 392 (1997).
[15] W. J. Ciccone, II, D. R. Bratton, D. M. Weinstein, and J. J. Elias, J. Bone Jt. Surg., Am. Vol. **88**, 1071 (2006).
[16] R. L. Lieber and T. J. Burkholder, *Biomedical Engineering Fundamentals*, The Biomedical Engineering Handbook No. 1, 3rd ed. (CRC Press, Boca Raton, Florida, 2006).
[17] J. Kastelic, A. Galeski, and E. Baer, Connect. Tissue Res. **6**, 11 (1978).
[18] J. Kastelic and E. Baer, Symp. Soc. Exp. Biol. **34**, 397 (1980).
[19] J. Kastelic, I. Palley, and E. Baer, J. Biomech. **13**, 887 (1980).
[20] S. L.-Y. Woo and D. J. Adams, in *Knee Ligaments: Structure, Function, Injury and Repair*, edited by D. Daniel, W. Akeson, and J. O'Connor (Raven Press, New York, 1990), Chap. 13, pp. 279–290.
[21] S. L.-Y. Woo, R. E. Debski, J. D. Withrow, and M. A. Janaushek, Am. J. Sports Med. **27**, 533 (1999).
[22] S. J. Eppel, B. N. Smith, H. Kahn, and R. Ballarini, J. R. Soc., Interface **3**, 117 (2006).
[23] F. H. Fu and S. B. Cohen, *Current Concepts in ACL Reconstruction*, 1st ed. (SLACK Inc., Thorofare, New Jersey, 2008).
[24] G. A. Livesay, T. W. Rudy, S. L.-Y. Woo, T. J. Runco, M. Sakane, G. Li, and F. H. Fu, J. Orthop. Res. **15**, 278 (1997).
[25] M. Sakane, R. J. Fox, S. L.-Y. Woo, G. A. Livesay, G. Li, and F. H. Fu, J. Orthop. Res. **15**, 285 (1997).