

Mechanical model for a collagen fibril pair in extracellular matrix

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Abstract In this paper, we model the mechanics of a collagen pair in the connective tissue extracellular matrix that exists in abundance throughout animals, including the human body. This connective tissue comprises repeated units of two main structures, namely collagens as well as axial, parallel and regular anionic glycosaminoglycan between collagens. The collagen fibril can be modeled by Hooke's law whereas anionic glycosaminoglycan behaves more like a rubber-band rod and as such can be better modeled by the worm-like chain model. While both computer simulations and continuum mechanics models have been investigated for the behavior of this connective tissue typically, authors either assume a simple form of the molecular potential energy or entirely ignore the microscopic structure of the connective tissue. Here, we apply basic physical methodologies and simple applied mathematical modeling techniques to describe the collagen pair quantitatively. We found that the growth of fibrils was intimately related to the maximum length of the anionic glycosaminoglycan and the relative displacement of two adjacent fibrils, which in return was closely related to the effectiveness of anionic glycosaminoglycan in transmitting

forces between fibrils. These reveal the importance of the anionic glycosaminoglycan in maintaining the structural shape of the connective tissue extracellular matrix and eventually the shape modulus of human tissues. We also found that some macroscopic properties, like the maximum molecular energy and the breaking fraction of the collagen, were also related to the microscopic characteristics of the anionic glycosaminoglycan.

Keywords Mathematical modeling · Connective tissue extracellular matrix · Hooke's law · Worm-like chain model · Molecular potential energy

Introduction

Structural polymers help to maintain the human body shape from large external tractions. Collagen occurs extensively in all animals and is the defining structural polymer, existing in the connective tissue extracellular matrix (CTs), for example, skin, cartilage and bone. It acts to support life against vigorous daily activities. CTs are bridged and bonded by anionic glycosaminoglycan GAGs, such as parallel rows of decoran, which are the only molecules in CTs apart from protein fibres that can be visualized by an electron microscope (Scott 1991, 1988; Svoboda et al. 1993). A pair of segments on neighboring collagen fibrils, which are linked by GAGs chains, is termed a shape module and must deform reversibly to preserve the general structure of the organism against various external stresses (Haverkamp et al. 2005). The axial tension is transmitted and opposed by protein fibres while compression is resisted by water-soluble polysaccharide GAGs, e.g. chondroitin sulphate. These GAGs transmit forces from the local area of molecules to global

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fibrils by converting compression into disseminated tensile stress (Scott 1975). The mechanics involving the collagen and the elastin fibril is well understood, i.e. they behave mainly like a Hookean spring in the low stress limit, but the elasticity of GAGs' molecules is still under intensive investigation (Burr 2002).

Numerous computational and continuum mechanical methodologies have been utilized to study the mechanics of such CTs (Redaelli et al. 2003; Akkus 2005; Fritsch and Hellmich 2007; Hellmich et al. 2004; Jager and Fratzl 2000; Ji and Gao 2004; Kotha and Guzelsu 2003; Wang and Qian 2006). However, most tend to ignore the microscopic details of CTs or assume a simple form of the molecular potential energy in order to make their models tractable. In particular, for a continuum mechanical approach, generally a homogeneous structure of CTs is assumed. Since the CTs comprise of collagen pairs, here we adopt basic physical concepts and simple mathematical techniques to investigate the mechanical properties of a single collagen pair. While utilizing a quadratic energy form for the collagen, we incorporate the statistical nature of GAGs into our model by utilizing the worm-like chain model, which has both theoretically and experimentally been proved to be applicable to wide ranges of bio-macromolecules including unstructured DNA, RNA, GAGs and polysaccharide (Haverkamp et al. 2005; Baumann et al. 2000; Rief et al. 1997, 1998; Oesterhelt et al. 1999). We note that our work may form a theoretical basis for experimentalists for their work on collagen pairs.

GAGs can go through conformational transitions, which are defined by the sudden elongation of bio-molecules due to the change in their atomic allocations without an increase in external forces. GAGs, e.g. pectinate, have two distinct chair structures, namely 4C_1 and 1C_4 (Barrows et al. 1995), separated by an energy barrier of approximately 11 kcal/mol (Joshi and Rao 1979). Moreover, there exists a boat conformation ${}^{1,4}B$ with an energy level of approximately 5–8 kcal/mol above the most stable 4C_1 chair energy (Dowd et al. 1994). In the low energy configuration, nature prefers the 4C_1 chair state over other possible states because it possesses the minimum energy configuration in comparison to other possible states. However, under an external stress, these polysaccharides can undergo two conformational transitions reversibly beyond some critical stresses (Marszalek et al. 1999). For example, amylose undergoes its first conformational transition when the applied force is around 200 pN and its second transition when the applied force is around 500 pN. However, some polysaccharides like pigskin DS only go through one transition, while other polysaccharides like poly-anionic HA, neutral methyl cellulose and poly-cationic chitosan undergo no transitions at all. The reason for

these conformational transitions is closely linked to the total number of axial or equatorial linkages existing in each pyranose ring (monosaccharide). It is evident that the glycosidic linkages may act as levers to generate a sufficient torque to undertake the work done, which is necessary to perform ring conformational transitions. Hence, only glycosidic linkages with axial linkages can generate enough torque to flip the levers beyond a given critical stress while equatorial linkages can not. For a more extensive treatment of the conformational transitions see Marszalek et al. (1999) for details. This phenomena provides a crucial step for a molecule to transform from the entropic region into the Hookean regime. Although the above interpretation of the kinking conformational changes is largely accepted by most researchers, there exists some other interpretations to explain these conformational transitions (Kuttel and Naidoo 2005).

This paper is divided into four sections. In “Theory”, we derive a mathematical model for CTs, while in “Numerical results and analysis”, numerical results and some extension work on CTs are developed. In the last section, we present some conclusions.

Theory

In this section, we consider some simple applied mathematical models for a collagen pair. Since CTs contain repeated units of collagen pairs, a collagen pair is denoted by a single unit of such repeated collagen pairs, which is illustrated in Fig. 1. While we model collagens utilizing Hooke's law, GAGs are modeled utilizing the worm-like chain model, which has carefully taken the entropic nature of the molecular chain into account. Due to the symmetry of CTs, we consider a pair of collagens with axial and regular GAGs in between, especially bone. In reality, to assemble such segments into a whole CTs is a challenging task owing to the complicated molecular interactions between fibrils. In addition, to simplify our study of external applied forces, which consist of both tensile and compressive forces, only the tensile stress is examined because GAGs can convert compression stress into tensile stress and hence the total tensile stress is assumed to be the vectorial sum of both tensile and compression forces.

A well constructed and stable collagen pair is assumed to maintain its structure by the attachment of GAGs, subject to at least a small perturbation due to molecular interactions between collagen–collagen, collagens–GAGs, thermal fluctuations, sudden shocks, etc. Suppose that we apply a tensile stress on one end of the collagen 1 (see Fig. 2), where this perturbation alters the mechanical structure of the collagen pair.

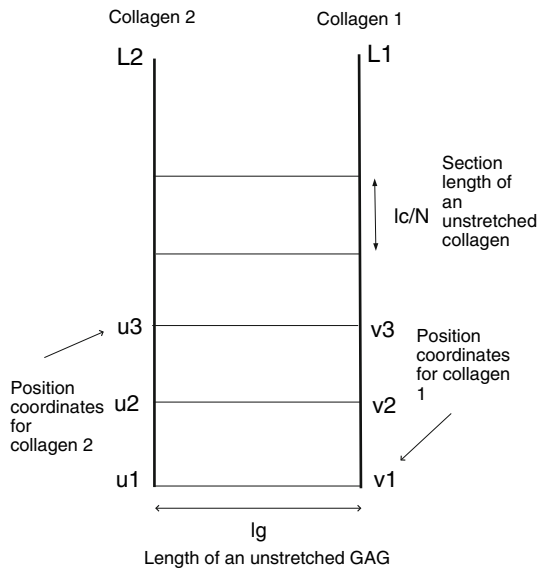


Fig. 1 Collagen pair before stretching, where L_1 and L_2 denote the collagens 1 and 2, respectively, $v_1 \dots v_N$ and $u_1 \dots u_N$ denote the position coordinates of oligomers in L_1 and L_2 , respectively, lc and lg are the natural lengths of the collagens and GAGs, respectively and N is the total number of oligomers that could exist in each collagen.

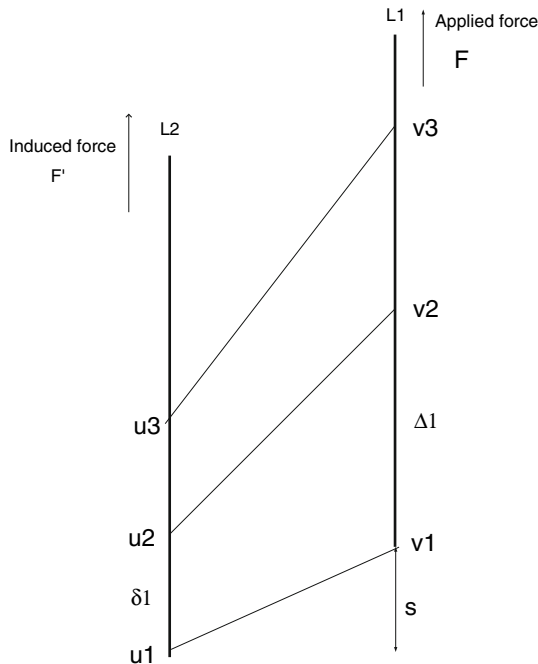


Fig. 2 Collagen pair after stretching, by an applied force F assumed to be acting on L_1 causing an induced force F' in L_2 , while s denotes the offset length between L_1 and L_2 , Δ_1 and δ_1 denote the length of the first oligomer in L_1 and L_2 , respectively, and so on

The displacements between v_{i+1} and v_i are denoted by Δ_i for $i = 1, \dots, N-1$ where N is the total number of oligomers, which are defined by a segment of the collagen pair

with two GAGs attached at its ends. Likewise for the collagen 2, the displacements of u_{i+1} and u_i are denoted by δ_i . Schematic diagrams of an un-stretched and a stretched collagen pair are shown in Figs. 1 and 2, respectively. We postulate the potential energy of collagens utilizing Hooke's law, which reads

$$V = \frac{1}{2} k \delta^2,$$

where k is a spring constant and δ is the extension. Given the potential energy form, it is straightforward to show that the potential energy of a collagen pair, V_c , is given by

$$V_c = \sum_{i=1}^N \frac{1}{2} k_c \left(\delta_i - \frac{\ell_c}{N} \right)^2 + \sum_{i=1}^N \frac{1}{2} k_c \left(\Delta_i - \frac{\ell_c}{N} \right)^2, \quad (1)$$

where N , k_c and ℓ_c are the total number of oligomers that exist in the collagen, the spring constant of the collagen, and the natural length of a collagen, respectively. Moreover, δ_i and Δ_i are defined by $\delta_i = u_{i+1} - u_i$ and $\Delta_i = v_{i+1} - v_i$ for $i = 1, 2, \dots, N-1$, respectively. In addition, we postulate the potential energy of GAGs utilizing the worm-like chain model. It is well-known that the interpolation force-extension formula for the worm-like chain model (Marko and Siggia 1995) is given by,

$$f = \frac{k_B T}{A} \left\{ \frac{z}{L} + \frac{1}{4} \left(1 - \frac{z}{L} \right)^{-2} - \frac{1}{4} \right\}, \quad (2)$$

where f , k_B , T , A , z , L denote the applied force, Boltzmann's constant, the absolute temperature, the persistence length, extension and the total contour length of the GAG, respectively. Then, the potential energy of all GAGs, V_g , can then be obtained by integrating Eq. 2 with respect to z and summing up the total number of GAGs, N , to yield

$$V_g = \sum_{i=1}^N \left\{ \frac{1}{2} k_g \left\{ \sqrt{(v_i - u_i)^2 + (\ell_g)^2} - \ell_g \right\}^2 + \frac{L^2}{4} k_g \left\{ 1 - \frac{\sqrt{(v_i - u_i)^2 + (\ell_g)^2} - \ell_g}{L} \right\}^{-1} - \frac{L}{4} k_g \left\{ \sqrt{(v_i - u_i)^2 + (\ell_g)^2} - \ell_g \right\} \right\}, \quad (3)$$

where k_g and ℓ_g denote $(k_B T)/(AL)$ and the natural length of GAGs, respectively. We can then relate u_i and v_i to δ_i , Δ_i and s , which is the off-set between fibrils (see Fig. 2). Notice that s is a function of f as the collagen pair starts to slide away with respect to each other, subject to the external force. Hence, u_i and v_i are geometrically related by

$$\begin{aligned}
v_1 &= u_1 + s, \\
v_2 &= u_2 + s + (\Delta_1 - \ell_c) - (\delta_1 - \ell_c) = u_2 + s + (\Delta_1 - \delta_1), \\
&\vdots \\
v_i &= u_i + s + \sum_{k=1}^i (\Delta_k - \delta_k), \\
&\vdots \\
v_N &= u_N + s + \sum_{k=1}^N (\Delta_k - \delta_k). \quad (4)
\end{aligned}$$

After we relate the kinematics between the collagen pair, we can simplify Eq. 3 in terms of the displacements δ_i and Δ_i , giving

$$\begin{aligned}
V_g &= \sum_{i=1}^N \left\{ \frac{1}{2} k_g \left\{ \sqrt{\left[s + \sum_{k=1}^i (\Delta_k - \delta_k) \right]^2 + (\ell_g)^2} - \ell_g \right\}^2 \right. \\
&\quad \left. + \frac{L^2}{4} k_g \left\{ 1 - \frac{\sqrt{\left[s + \sum_{k=1}^i (\Delta_k - \delta_k) \right]^2 + (\ell_g)^2} - \ell_g}{L} \right\}^{-1} \right. \\
&\quad \left. - \frac{L}{4} k_g \left\{ \sqrt{\left[s + \sum_{k=1}^i (\Delta_k - \delta_k) \right]^2 + (\ell_g)^2} - \ell_g \right\} \right\}. \quad (5)
\end{aligned}$$

Since the elongation of collagen 1 causes the elongation of collagen 2, we can relate δ_i and Δ_i by the relative displacements ε_i . That is

$$\Delta_i = \delta_i + \varepsilon_i. \quad (6)$$

Assuming statistical equilibrium, we let $\delta_i = \delta$, $\Delta_i = \Delta$ and $\varepsilon_i = \varepsilon$ for all i . Hence, Eqs. 1 and 5 reduce to

$$\begin{aligned}
V_c &= \frac{1}{2} k_c N \left\{ \left(\delta - \frac{\ell_c}{N} \right)^2 + \left(\delta + \varepsilon - \frac{\ell_c}{N} \right)^2 \right\}, \\
V_g &= \sum_{i=1}^N \left\{ \frac{1}{2} k_g \left\{ \sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g \right\}^2 \right. \\
&\quad \left. + \frac{L^2}{4} k_g \left\{ 1 - \frac{\sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g}{L} \right\}^{-1} \right. \\
&\quad \left. - \frac{L}{4} k_g \left\{ \sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g \right\} \right\}. \quad (7)
\end{aligned}$$

Since each GAG has its own maximum length K and the displacement between u_N and v_N corresponds the maximum length of GAG given in the collagen pair, which must be smaller or equal to K . Given that, we have

$$|v_N - u_N| = \sqrt{(s + N\varepsilon)^2 + (\ell_g)^2} \leq K, \quad (8)$$

from which, we show that the maximum number of oligomers N_{\max} allowed in a given collagen satisfies the following inequality

$$N_{\max} \leq \frac{\sqrt{(K)^2 - (\ell_g)^2} - s}{\varepsilon} = \left\lfloor \frac{\sqrt{(K)^2 - (\ell_g)^2} - s}{\varepsilon} \right\rfloor, \quad (9)$$

where $\lfloor \cdot \rfloor$ denotes minimum integer value of the enclosed real number, e.g. $\lfloor 4.3 \rfloor = 4$, respectively. Note that Eq. 9 ignores the maximum strain that can be held by a collagen, and while ε is a rather abstract quantity, it can be expressed in terms of s by minimizing the maximum potential energy E_{\max} of the collagen pair with respect to ε at equilibrium (see Appendix for details). At first glance, s is insignificant under small natural external forces, i.e. thermal fluctuations and internal molecular interactions. However, s becomes crucial when we consider the collagen pair under large external tractions. One interesting thing about the above equation is that it limits the possible number of oligomers that can exist for a given stable collagen and it is model independent because it arises solely from a geometric point of view. Also, the inequality reveals the importance of GAGs in relation to the growth of the collagen pair. Hence, the longer the maximum length of GAGs, the longer the structural collagen pair can be. Although the inequality does not prove the possibility of the existence of ring conformational transitions of GAGs, it does provide evidence that the existence of conformational transitions increases K and hence encourages the growth of the collagen pair. Further, the higher the effectiveness of the force transmission of GAGs between fibril and fibril, the lower the value of ε , and hence longer the collagen can be.

The induced force, F' , in collagen 2, generated by collagen 1 and the relative displacement, ε , of the system, can be determined to be

$$F' = F - k_c \varepsilon, \quad \varepsilon = \frac{1}{N} (L_1 - L_2), \quad (10)$$

where L_1 and L_2 are the total molecular contour length of the collagen 1 and 2, respectively. F' and ε can hence be determined experimentally by knowing k_c , F , N , L_1 and L_2 . In particular, ε can be measured to find N_{\max} . Given N_{\max} , we can obtain the maximum molecular energy for a collagen pair, E_{\max} , namely

$$\begin{aligned}
E_{\max} &= \frac{1}{2} k_c N_{\max} \left\{ \left(\delta - \frac{\ell_c}{N_{\max}} \right)^2 + \left(\delta + \varepsilon - \frac{\ell_c}{N_{\max}} \right)^2 \right\} \\
&\quad + \sum_{i=1}^{N_{\max}} \left\{ \frac{1}{2} k_g \left\{ \sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g \right\}^2 \right. \\
&\quad \left. + \frac{L^2}{4} k_g \left\{ 1 - \frac{\sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g}{L} \right\}^{-1} \right. \\
&\quad \left. - \frac{L}{4} k_g \left\{ \sqrt{(s + i\varepsilon)^2 + (\ell_g)^2} - \ell_g \right\} \right\}. \quad (11)
\end{aligned}$$

The maximum molecular energy E_{\max} grows quadratically with the extension δ and is related linearly to N_{\max} , which

is given by Eq. 9 and determined by K and ε . Hence, the existence of flexible GAGs with long maximum length K increases the number of oligomers N_{\max} , which in return tightens the system dramatically. In addition, assuming a large N_{\max} and a small ε , the modulus of a collagen pair, k_t , can be determined easily by the second derivative of E_{\max} with respect to δ . Upon performing two differentiations, we approximate the modulus of the collagen pair, k_t , as

$$k_t \approx k_c N_{\max}. \quad (12)$$

Again, k_t depends linearly on N_{\max} , where the rest of arguments are very similar to the discussion for the maximum molecular energy above.

Numerical results and analysis

In this section, we carry out a numerical analysis on the results derived in the previous section, and finally we examine the breaking point of a collagen pair. Firstly, given Eq. 11, we assume the value of the parameters given in Redaelli et al. (2003), namely $k_c = 0.2$ GPa, $k_g = 0.02$ GPa, $\ell_c = 100$ μm , $\ell_g = 0.02$ nm, $L = 0.2$ nm and 3 maximum numbers of oligomer are examined, namely $N_{\max1} = 1$ K, $N_{\max2} = 10$ K and $N_{\max3} = 0.1$ M. Further, without loss of generality, the offset s is assumed to be zero, which corresponds to the tight molecular interaction between fibrils or the collagen pair under a small traction. The potential energy of GAGs is neglected due to its insignificance in comparison to the potential energy of the collagen pair that is demonstrated in Fig. 3, where ε has been linearized with the extension δ . The numerical result shows that the potential energy of GAGs utilizing the above parameters is 6 orders of magnitude

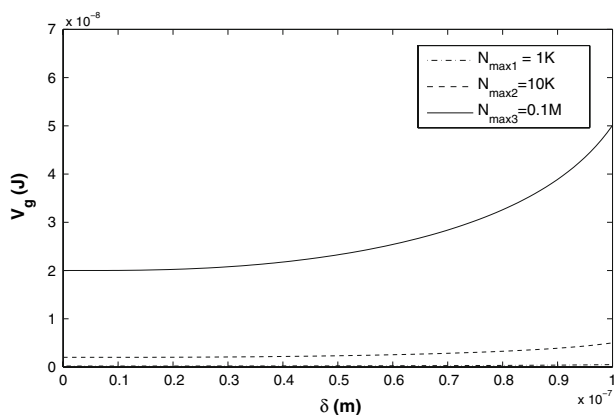


Fig. 3 Potential energy of GAG, V_g , versus extension, δ ranging from 0 to 100 nm, for $N_{\max1} = 1$ K, $N_{\max2} = 10$ K and $N_{\max3} = 0.1$ M respectively

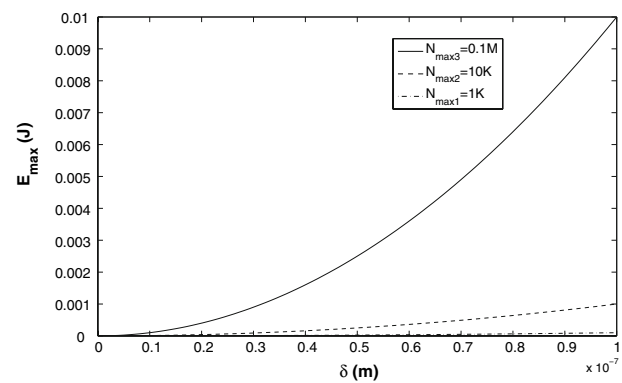


Fig. 4 Potential energy of the collagen pair, E_{\max} , versus extension, δ ranging from 0 to 100 nm, for $N_{\max1} = 1$ K, $N_{\max2} = 10$ K and $N_{\max3} = 0.1$ M, respectively

smaller than the potential energies of the paired collagen for all three cases we considered. Given that, the potential energies of the collagen pair versus the extension δ , ranging from 0 to 100 nm for $N_{\max1}$, $N_{\max2}$ and $N_{\max3}$, are plotted together in Fig. 4.

Note that the maximum molecular energy increases quadratically when the extension increases linearly. In addition, δ is determined by the applied force F and the relative displacement ε . For example, for a constant Δ , δ achieves its maximum value when $\varepsilon = 0$. Further, E_{\max} increases linearly with N_{\max} , which in return depends positively on K but negatively on ε . The toughness of a collagen pair, k_t , is defined in the previous section as the second derivative of E_{\max} with respect to δ , and hence the higher the slope of E_{\max} with respect to the extension δ , the stiffer the collagen pair is. In conclusion, given a collagen pair, it is tougher whenever GAGs have a higher value of K and a higher ability in transmitting forces between fibrils. However, the existence of GAGs contributes almost nothing to the toughness of the collagen pair but is significant to maintain the stable structure and boost up the toughness of the collagen pair, which are consistent to the results that an increased PYD or DPD ratio (the most abundant mature GAGs in bone collagen) is related to the increased compressive strength in bone (CTs) (Lees et al. 1990; Bailey et al. 1992; Oxlund et al. 1995, 1996; Banse et al. 2002) but has no huge effect on toughness or ductility of bone (Zioupou et al. 1999; Wang et al. 2002; Keaveny et al. 2003; Hernandez et al. 2005).

We end this section by extending concepts that we developed above to determine the point at which a collagen pair will break. For the study of a collagen pair, an important parameter is the fraction of the collagen pair, χ_R , in which the breaking point occurs (see Fig. 5). The breaking point is assumed to occur when the bridge

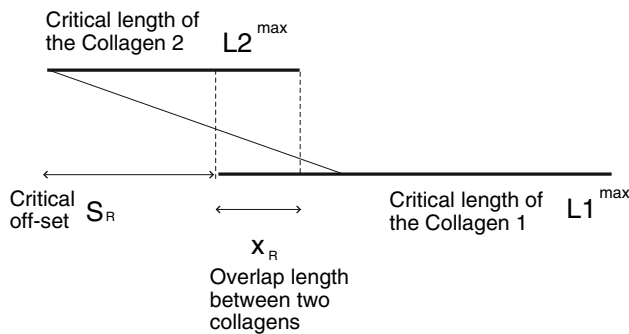


Fig. 5 The breaking fraction of the collagen pair

between u_1 and v_1 is finally broken (see Figs. 1, 2). From Fig. 5, we write

$$L_1^{\max} + L_2^{\max} - \chi_R = s_R + L_1^{\max}, \quad (13)$$

where L_1^{\max} and L_2^{\max} are the critical lengths of collagens 1 and 2, respectively and s_R is the critical off-set of the system. After some re-arrangement, we found that

$$\chi_R = L_2^{\max} - s_R. \quad (14)$$

In addition, we know that when the collagen pair was about to be torn apart, $N_{\max} = 0$, from Eq. 9, we deduce

$$s_R = \sqrt{(K)^2 - (\ell_g)^2}. \quad (15)$$

Therefore, upon comparing Eqs. 14 and 15, we have

$$\chi_R = L_2^{\max} - \sqrt{(K)^2 - (\ell_g)^2}. \quad (16)$$

Notice that the above equation links the macro-quantity χ_R to micro-quantities such as L_2^{\max} , K and ℓ_g . Once again, the larger the possible length of GAGs, the smaller the breaking fraction of the collagen pair, which implies that we need to put more forces in the system to tear the collagen pair apart, which is consistent to the theoretical result obtained by Buehler (2006).

Conclusion

In this paper, we utilize simple applied mathematical modeling techniques, for example Hooke's law, to describe the structure of a collagen pair. We found that for maintaining the stability of a collagen pair, the maximum number of oligomers that can exist in a given collagen depends on the maximum length of GAGs and the effectiveness of the GAGs in transferring forces between fibrils. That is, a collagen can grow longer for the longer GAGs and the higher effectiveness of GAGs in transferring forces between fibrils. This concept can then

be extended naturally to the toughness and the breaking point of a collagen pair, which are found to be intimately related to the characteristics of GAGs. In addition, the possible conformational transitions of GAGs strengthen the whole structure of CTs and as such CTs maintain our body shape from any large external traction. We note that our work does not give the complete picture where a more sophisticated theoretical investigation of the interactions between collagens and GAGs needs to be undertaken and extend our model to investigate the mechanical properties of CTs. In addition, we sincerely refer our readers, who are interested in utilizing computing simulations and continuum mechanics to model the macroscopic structure of CTs, to those references listed in the "Introduction".

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Appendix

Obtaining ε from minimization

From Eq. 11, if N_{\max} is sufficiently large, then we can approximate the summation by integration. Upon utilizing equation Eq. 9, we obtain

$$\begin{aligned} E_{\max} = & \frac{1}{2}k_c \left(\frac{\Phi - s}{\varepsilon} \right) \left\{ \left(\delta - \frac{\ell_c}{\Phi - s} \varepsilon \right)^2 \right. \\ & + \left[\delta + \left(1 - \frac{\ell_c}{\Phi - s} \right) \varepsilon \right]^2 \left. \right\} \\ & + \int_0^{\frac{\Phi - s}{\varepsilon}} \frac{1}{2}k_g \left\{ \sqrt{(s + \varepsilon x)^2 + \ell_g^2} - \ell_g \right\}^2 dx \\ & + \int_0^{\frac{\Phi - s}{\varepsilon}} \frac{L^2}{4}k_g \left\{ 1 - \frac{\sqrt{(s + \varepsilon x)^2 + \ell_g^2} - \ell_g}{L} \right\}^{-1} dx \\ & - \int_0^{\frac{\Phi - s}{\varepsilon}} \frac{L}{4}k_g \left\{ \sqrt{(s + \varepsilon x)^2 + \ell_g^2} - \ell_g \right\} dx, \end{aligned} \quad (17)$$

where $\Phi = \sqrt{K^2 - \ell_g^2}$. If we substitute $s + \varepsilon x = \ell_g \tan \theta$ and perform the integration, we obtain

$$\begin{aligned} E_{\max} = & \frac{1}{2}k_c \left(\frac{\Phi - s}{\varepsilon} \right) \left\{ \left(\delta - \frac{\ell_c}{\Phi - s} \varepsilon \right)^2 \right. \\ & + \left[\delta + \left(1 - \frac{\ell_c}{\Phi - s} \right) \varepsilon \right]^2 \left. \right\} + \frac{H(s)}{\varepsilon}, \end{aligned} \quad (18)$$

where $H(s) = (1/2)k_g \ell_g^3 a(s) + (L^2/4)k_g \ell_g b(s) - (L/4)k_g \ell_g^2 c(s)$ and

$$\begin{aligned}
a(s) &= 2 \tan \theta + (1/3) \tan^3 \theta - \tan \theta \sec \theta \\
&\quad - \ln(\sec \theta + \tan \theta) \Big|_{\arctan(s/\ell_g)}^{\arctan(\Phi/\ell_g)}, \\
b(s) &= -\frac{L \ln[\tan \frac{\theta}{2} + 1]}{\ell_g} + \frac{L \ln[\tan \frac{\theta}{2} - 1]}{\ell_g} \\
&\quad + 2L \left(1 + \frac{L}{\ell_g}\right) \frac{\arctan \left[\frac{(L+2\ell_g) \tan \frac{\theta}{2}}{\sqrt{L(L+2\ell_g)}} \right]}{\sqrt{L(L+2\ell_g)}} \Big|_{\arctan(s/\ell_g)}^{\arctan(\Phi/\ell_g)}, \\
c(s) &= \frac{1}{2} \tan \theta + \frac{1}{2} \ln(\tan \theta + \sec \theta) - \tan \theta \Big|_{\arctan(s/\ell_g)}^{\arctan(\Phi/\ell_g)}. \quad (19)
\end{aligned}$$

We note that the energy form given in Eq. 18 might be utilized to carry out computer simulations or global mathematical modelings for CTs in a more accurate way. To find the minimum value of E_{\max} with respect to ε , we require $\partial E_{\max} / \partial \varepsilon = 0$. Given that, we have

$$\varepsilon = \sqrt{\frac{2 \left[\delta^2 + \frac{H}{k(\Phi-s)} \right]}{\left(\frac{\ell_c}{\Phi-s} \right)^2 + \left(1 - \frac{\ell_c}{\Phi-s} \right)^2}}. \quad (20)$$

Upon knowing s , ε can be easily solved from the above equation.

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