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Two-scale hyperelastic model of a material with prestress at cellular level

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Abstract

We propose the two-scale hyperelastic model of a material defined at micro-scale. The microstructure, motivated by the arrangement of soft tissues at the cellular level, is formed by an incompressible inclusion and linear elastic elements. The prestress of such structure is maintained by the assumption of constant volume of the inclusion. In the continuum limit, the prestressed microstructure is considered as a single material particle governed by the macroscopic deformation gradient. Thus the strain-energy is obtained as a function of both macro-deformation and micro-prestress. Although we have no analytical formula, an approximation is found using assumptions that hold for soft tissues. It shows clearly the ability of the model to control the overall mechanical behaviour by setting the prestress at micro-scale (the prestress-induced stiffening).

Keywords: multi-scale modelling, prestress, soft tissue

1. Introduction

The prestress (pre-existing stress in unloaded state) is present within many materials, and it is also a common feature in technical practice. Although it plays an important role in mechanical response, it is difficult to include prestress into classical material models. It motivates us to propose more complex material models with the prestress arising from the arrangement of their microstructure. The main motivation comes from biological tissues. As experimentally observed [2, 11], the fibres within living cells carry the prestress which plays an important role in cell mechanics. By increasing its prestress, the cell increases its stiffness (the so-called prestress-induced stiffening [10]), and thus controls actively the behaviour of the whole tissue. The muscle contraction, for instance, is accompanied by a change in the rest lengths of cell fibres, i.e. by a change of its prestress. At the cell level, this behaviour is successfully described by the idea of tensegrity [3, 6, 12] where the cytoskeleton is modelled as a prestressed structure using cables and struts. Tension in cables is balanced by the compression in struts and thus a stable structure is created. Although it explains a lot of features of adherent cells [7], it is less clear how to implant tensegrity idea into a macroscopic model of living tissues.

Therefore we propose another approach of balancing the tension based on the fact that cells maintain a constant volume [8]. We consider the constant volume of a cell as a constraint which does not allow the inner fibers to relax. This idea is applied in [9] to develop a model of a prestressed living cell. It exhibits the prestress-induced stiffening which is proved by deriving the formula of Young's modulus.

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In this paper, we use the model of microstructure proposed in [9] to develop a two-scale hyperelastic model of a prestressed material motivated by a soft tissue. We are aware, that considering a soft tissue as a hyperelastic material is a drastic simplification of reality. The setting is purely isothermal, all the chemistry is neglected, and the response is path-independend, i.e. without viscous effects [1, 5]. Therefore, hyperelastic models are not capable of describing real tissues and serve as a rough approximation. However, it is possible to focus on some aspects of tissue behaviour arising from the arrangement of its microstructure. Embedding these aspects into hyperelastic models helps to understand how changes at micro-scale affect the overall mechanical response.

Such approach is used in [4] to propose the hyperelastic model of a material which microstructure is formed by balls and springs. Using linear elastic elements, a simple mechanical model of a living cell reinforced by cytoskeleton with a surrounding extracellular matrix is created. Considering this structure as a single continuum point, the macroscopic model is developed which material parameters are related transparently to the arrangement of microstructure. Although it is not an accurate model of real tissue, it allows to understand how certain features (such as cell-matrix volume ratio, rigidity ratio, anisotropy) affect the overall macroscopic behaviour.

The aim of this work is to extend the model developed in [4] using the prestressed microstructure proposed in [9]. The resulting hyperelastic model is orthotropic, it respects the microstructure of the soft tissue via the simple mechanic model of living cell, and it allows to study the effect of the cell prestress at the macro-scale. Although there is no analytical formula of strain-energy function, an approximation suitable for soft tissues is found. The ability of the model to control the overall macroscopic behaviour by setting the prestress is demonstrated on the simple traction test. The paper is organized as follows.

In section 2, the microstructure at the level of living cell is defined. Using an assumption of the cell constant volume, the determination of the reference state is equivalent to the solution of minimization problem with constraint. It gives rise to the prestress that is transparently quantified by additional parameters.

In section 3, the strain energy function of the model is determined using a direct micro-macro passage (an RVE concept). An approximate analytical formula suitable for soft tissues is found. It is an explicit function of both deformation and prestress.

The Young's modulus is determined in section 4. At the micro-scale, it represents the stiffness of an individual living cell. Using the approximate formula, the prestress-induced stiffening observed for living cells is shown.

The simple traction test is performed in section 5, showing the dependence on prestress. The ability of the model to control its macroscopic behaviour via setting the prestress at micro-level is thus shown.

2. The microstructure of the model

A body is considered as a two-scale continuum. In our approach it means that each material point $\boldsymbol{X}$ of the macroscopic body Ω in reference configuration is connected with a representative volume element (RVE) on which the microstructure is defined, see Fig. 1. In this case, RVE consists of a living cell and an extracellular matrix that are both modelled using linear elastic elements. Let us denote the principal spatial directions with $i = 1, 2, 3$. The living cell is then modelled as a ball of ellipsoid shape with dimensions c_i^{ref} filled with an incompressible fluid. The cytoskeleton, which reinforces the cell, is represented by linear springs with rigidities

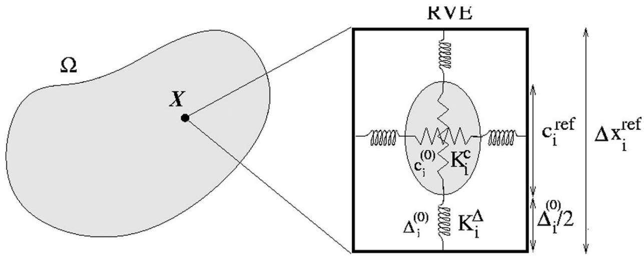

Fig. 1. The reference configuration. Each continuum point is considered as an RVE with defined microstructure

K_i^c and rest lengths $c_i^{(0)}$. The cell is surrounded by an extracellular matrix which elasticity is represented by linear springs with rigidities K_i^Δ and rest lengths $\Delta_i^{(0)}$. We consider the periodicity of microstructure, i.e. each ball is connected with six other balls (two for each spatial direction), and the gap between two balls is $\Delta_i^{(0)}$ in each spatial direction (the extracellular matrix is assumed to be relaxed at reference state). Consequently, it is

$$\Delta x_i^{ref} = c_i^{ref} + \Delta_i^{(0)}\,, \tag{1}$$

where Δx_i^{ref} is the size of RVE in reference state in i-th direction.

The crucial assumption is that the constant volume of the ball, V_{ball}, does not allow inner springs to take their rest lengths $c_i^{(0)}$. Introducing $V_c = c_1^{ref} c_2^{ref} c_3^{ref}$, the assumption means that the conditions

$$V_c = \text{const}\,, \quad V_c \neq c_1^{(0)} c_2^{(0)} c_3^{(0)}\,, \tag{2}$$

are fulfilled (notice that $V_{ball} = \frac{\pi}{6} V_c$). Consequently, there is a pre-existing tension within the inner springs that can be described by the prestress (prestrain) parameter,

$$P_i = 1 - \frac{c_i^{(0)}}{c_i^{ref}}, \tag{3}$$

for each spatial direction. For the tensional prestress, it is $P_i \in [0, 1)$, where $P_i = 0$ represents the structure with no prestress ($c_i^{ref} = c_i^{(0)}$), whereas $P_i \to 1$ is the limit value representing the maximum possible prestress ($c_i^{ref} \neq 0$, $c_i^{(0)} \to 0$).

However, the parameters P_i are not independent. Concerning the ball, there are 7 parameters, V_c, c_i^{ref}, and $c_i^{(0)}$, and only 4 of them are independent. For example, if the volume V_c and the rest lengths $c_i^{(0)}$ are given, the ball occupies such shape (determined by c_i^{ref}) so that the elastic energy stored in the inner springs is minimal. It is equivalent to the fact that there are no outer forces in reference state and the prestress is maintained only by the constant volume of the ball. The energy of the ball in the reference configuration is

$$E_{ball}^{ref} = \sum_{i=1}^{3} \frac{K_i^c}{2} \left(c_i^{ref} - c_i^{(0)} \right)^2 . \tag{4}$$

Minimization of E_{ball}^{ref} with respect to c_i^{ref} is equivalent to finding the stationary point of a Lagrange function defined as

$$L(c_1^{ref}, c_2^{ref}, c_3^{ref}, \lambda) = E_{ball}^{ref} + \lambda (c_1^{ref} c_2^{ref} c_3^{ref} - V_c)\,, \tag{5}$$

where λ is a Lagrange multiplier. It leads to the set of equations

$$\begin{aligned} K_1^c\left(c_1^{ref}-c_1^{(0)}\right)+\lambda c_2^{ref}c_3^{ref} &= 0\\ K_2^c\left(c_2^{ref}-c_2^{(0)}\right)+\lambda c_1^{ref}c_3^{ref} &= 0\\ K_3^c\left(c_3^{ref}-c_3^{(0)}\right)+\lambda c_1^{ref}c_2^{ref} &= 0\\ c_1^{ref}c_2^{ref}c_3^{ref}-V_c &= 0\,, \end{aligned} \tag{6}$$

which must always hold. The solution are the parameters c_i^{ref} and consequently the prestress parameters P_i.

In the terms of prestress, the set (6) leads to the conditions

$$\frac{P_i}{P_j}\left(\frac{c_i^{ref}}{c_j^{ref}}\right)^2\frac{K_i^c}{K_j^c}=1\,,\quad i\neq j\,, \tag{7}$$

which are more useful. In what follows, we consider that the known parameters are c_i^{ref}, and one chosen prestress parameter, e.g. $P_1 \neq 0$. The rest two parameters, here P_2, and P_3, are then determined by the relations (7) which express the energy minimizing condition.

3. Strain-energy function

3.1. Micro-macro passage

The passage from micro- to macro-scale is very straightforward in our approach. We assume that the shape of RVE connected with a particle $\boldsymbol{X}$ is governed directly by the macroscopic deformation gradient, $\mathbf{F}(\boldsymbol{X})$. Let us consider the deformation states $\boldsymbol{\varphi}(\Omega)$ with diagonal deformation gradient,

$$\mathbf{F}(\boldsymbol{X})=\begin{pmatrix}\beta_1 & 0 & 0\\ 0 & \beta_2 & 0\\ 0 & 0 & \beta_3\end{pmatrix}. \tag{8}$$

The sizes of RVE corresponding to the point $\boldsymbol{x}=\boldsymbol{\varphi}(\boldsymbol{X})$ are then given as

$$\Delta x_i=\beta_i\Delta x_i^{ref}\,, \tag{9}$$

which is depicted in Fig. 2.

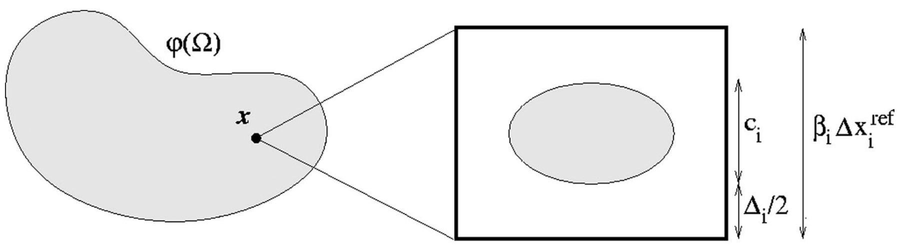

Fig. 2. The deformed configuration. Deformation of the RVE in spatial direction i is governed by the element β_i of macroscopic deformation gradient

Notice that the deformation gradient does not determine the shape of the ball within RVE, c_i, which is treated as an inner degree of freedom. In our approach we assume that it is determined by the energy minimizing principle. In other words, the macroscopic deformation gradient sets the boundary of RVE, and the microstructure occupies such configuration which minimizes its energy, namely

$$E_{RVE} = \min_{\substack{c_i \\ c_1 c_2 c_3 = V_c}} \sum_{i=1}^{3} \left[\frac{K_i^c}{2} \left(c_i - c_i^{(0)} \right)^2 + \frac{K_i^\Delta}{2} \left(\Delta_i - \Delta_i^{(0)} \right)^2 \right] . \tag{10}$$

Here,

$$\Delta_i = \Delta x_i - c_i \, . \tag{11}$$

At the macro-scale, the strain-energy function is determined as the elastic energy per unit volume. Due to the direct micro-macro passage, it is

$$W_{BS} = \frac{E_{RVE}}{V_{RVE}} \, , \tag{12}$$

where V_{RVE} is the volume of the RVE at reference state. Using (3), and (9), the strain-energy can be expressed as a function of both macroscopic deformation gradient and microscopic prestress. Namely,

$$W_{BS}(\mathbf{F}, P_i) = W_{spring}(\mathbf{F}, P_i) + W'(\mathbf{F}, P_i) \tag{13}$$

$$W_{spring} = \frac{1}{2V_{RVE}} \sum_{i=1}^{3} B_i \left(\Delta x_i^{ref} (\beta_i - 1) + c_i^{ref} P_i \right)^2 \tag{14}$$

$$W' = \frac{V_c^{2/3}}{2V_{RVE}} \min_{\substack{r_i \\ r_1 r_2 r_3 = 1}} \sum_{i=1}^{3} A_i (r_i - q_i)^2 \, . \tag{15}$$

Here,

$$B_i = K_i^c (1 + k_i)^{-1} \, , \quad k_i = \frac{K_i^c}{K_i^\Delta} \, , \quad A_i = K_i^c + K_i^\Delta \, , \quad r_i = \frac{c_i}{V_c^{1/3}} \, . \tag{16}$$

The parameters $q_i = q_i(\beta_i, P_i)$ are the bilinear functions,

$$q_i = \frac{c_i^{ref}}{V_c^{1/3}} \beta_i^{eff} \, , \quad \beta_i^{eff} = \frac{1 + \delta_i}{1 + k_i} (\beta_i - 1) + 1 - \frac{k_i}{1 + k_i} P_i \, , \quad \delta_i = \frac{\Delta_i^{(0)}}{c_i^{ref}} \, . \tag{17}$$

It is worth stressing that throughout this paper, both microscopic and macroscopic incompressibility are assumed. The microscopic incompressibility, which represents the assumption of the cell constant volume, relates the dimensions of inner ball, whereas the macroscopic incompressibility relates the elements of deformation gradient. The relations

$$r_1 r_2 r_3 = 1 \, , \quad \beta_1 \beta_2 \beta_3 = 1 \, , \tag{18}$$

thus always hold causing a non-linear behaviour at the both micro- and macro-scale.

3.2. The approximate formula

It is impossible to solve the minimizing problem (15) analytically. The expression of strain-energy function (13) can thus be used only for the numerical simulations where the minimization is proceeded in each node of computational mesh. For larger problems, this can be very time consuming. Moreover, an analytical formula is necessary to study the influence of prestress on the macroscopic mechanical behaviour. Fortunatelly, it is possible to find an approximation that is suitable for soft tissues.

Assume that the solution of (15) can be written in the form

$$r_i = q_i + \varepsilon_i\,, \quad \varepsilon_i \ll q_i\,. \tag{19}$$

Neglecting the second and higher powers of ε_i, we obtain the following formula,

$$W' \approx \frac{1}{2}\frac{V_c^{2/3}}{V_{ref}}\frac{A_1A_2A_3(1-q_1q_2q_3)^2}{A_1A_2q_1^2q_2^2 + A_2A_3q_2^2q_3^2 + A_1A_3q_1^2q_3^2}\,. \tag{20}$$

Thus the hyperelastic material with the explicit dependency of strain-energy function on both deformation and prestress can be introduced

$$\begin{aligned} W_{bs}(\mathbf{F}, P_i) \;=\;& \frac{1}{2V_{RVE}}\sum_{i=1}^{3} B_i\left(\Delta x_i^{ref}(\beta_i - 1) + c_i^{ref}P_i\right)^2 + \\ &+\frac{1}{2}\frac{V_c^{2/3}}{V_{ref}}\frac{A_1A_2A_3(1-q_1q_2q_3)^2}{A_1A_2q_1^2q_2^2 + A_2A_3q_2^2q_3^2 + A_1A_3q_1^2q_3^2}\,, \end{aligned} \tag{21}$$

which approximates the behaviour of the "balls and springs" model. The accuracy of this approximation is given by the condition

$$q_1q_2q_3 \approx 1\,, \tag{22}$$

ensuring that (19) holds (notice that $r_i = q_i$ for $q_1q_2q_3 = 1$). Employing (17), (22) can be rewritten in the form

$$\beta_1^{eff}\beta_2^{eff}\beta_3^{eff} \approx 1\,. \tag{23}$$

For arbitrary β_i and P_i, the condition (23) is fulfilled for

$$k_i \ll 1\,, \quad \delta_i \approx k_i\,, \tag{24}$$

since it implies

$$\beta_1^{eff}\beta_2^{eff}\beta_3^{eff} \approx \beta_1\beta_2\beta_3 = 1\,. \tag{25}$$

Fortunately, (24) is a reasonable assumption for the case of soft tissues (especially for smooth muscles). The left-hand inequality means that the living cell is much softer than the extracellular matrix. The right-hand approximation means that the volume of RVE is almost completely filled by living cell and only a little space is occupied by extracellular matrix. Both assumptions meet biological observations.

4. Young's modulus

Consider the transverse isotropy, i.e. the material parameters are the same in the spatial directions $i = 2, 3$. The prestress is set via the parameter P_1, the parameter P_2 is consequently determined by (7). Applying a small deformation ε in the direction $i = 1$, it is

$$\beta_1 = 1 + \varepsilon \,, \quad \beta_2 = \beta_3 = (1 + \varepsilon)^{-1/2} \,. \tag{26}$$

The strain-energy (13) is thus a function $W = W(\varepsilon, P_1)$ and the corresponding Young's modulus can be determined as

$$Y_{BS}(P_1) = \left. \frac{\mathrm{d}^2 W_{BS}(\varepsilon, P_1)}{\mathrm{d}\varepsilon^2} \right|_{\varepsilon=0} . \tag{27}$$

Due to the straightforward micro-macro passage (12), the Young's modulus of the macroscopic model is in fact the Young's modulus of a single RVE. The function $Y_{BS} = Y_{BS}(P_1)$ thus expresses the dependence of the stiffness of the individual cell with surrounding extracellular matrix on its prestress. The equation (27) cannot be solved analytically, therefore we consider the approximation

$$Y_{bs}(P_1) = \left. \frac{\mathrm{d}^2 W_{bs}(\varepsilon, P_1)}{\mathrm{d}\varepsilon^2} \right|_{\varepsilon=0} , \tag{28}$$

which was already found in [9]. Using the notation (16), it can be written in the form

$$Y_{bs}(P_1) = Y_0 \left[1 + f \cdot P_1 \right] , \tag{29}$$

where Y_0 is the Young's modulus of the structure with no prestress, and f is a function of material parameters. Namely,

$$\begin{aligned} f \; = \; & \frac{3k_1B_1}{b^2} \frac{4A_1^2(1+k_1)^2h^2 + 8A_1(1+k_1)hb[A_2(1+k_1)hb - A_1(1+k_2)] +}{(1+k_1)(1+k_2)(2A_1 + A_2b^2)[2A_2B_1(1+k_1)(1+k_2)b^2 +} \cdots \\ & \frac{+b^2[A_2^2(1+k_1)^2h^2b^2 - 12A_1A_2(1+k_1)(1+k_2)hb + 8A_1^2(1+k_2)^2] +}{+2A_2B_1(1+k_1)^2h^2 + A_2B_2k_1(1+k_2)h^2b^2 - 4A_2B_1(1+k_1)hb +} \\ & \frac{+8A_1A_2(1+k_2)^2b^4}{+4A_1B_1k_1(1+k_2)]} \,, \end{aligned} \tag{30}$$

where $h = \Delta x_2^{ref}/\Delta x_1^{ref}$, and $b = c_2^{ref}/c_1^{ref}$. Although f is a complicated function, it is always $0 < f < 1$ and it is not dependent on pretress. The relation (29) thus clearly expresses the dependence of the cell stiffness on its prestress, the so-called prestress-induced stiffening, that is observed for living cells.

It is worth stressing that in the isotropic case, i.e. the parameters are the same in all three directions, the function f is simplified into

$$f_{iso} = \frac{1}{1 + k_1} \,. \tag{31}$$

The assumption (24), i.e. $k_i \to 0$, implies $f_{iso} \to 1$, i.e. the model exhibits the most significant dependency on prestress. When the prestress is set to its limit value, $P_1 = 1$, the stiffness of the material is doubled. Such case is considered in Fig. 3, where the dependency of the Young's modulus on the prestress for both approximate, Y_{bs}, and exact formula, Y_{BS}, is plotted. The assumptions (24) ensure a good accuracy.

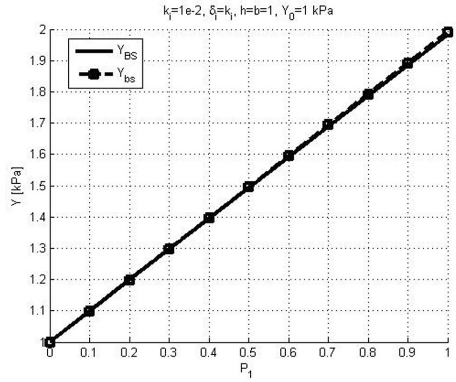

Fig. 3. Prestress-induced stiffening. The numerical formula, Y_{BS}, is represented by the solid line. The analytical approximate formula, Y_{bs}, is depicted by the dashed line with squares

5. Traction test

To show the dependence of the material's behaviour on the prestress in the regime of large deformation, let us perform a simple traction test. The transverse isotropy is assumed as in the previous section, and the prestress is set via the parameter P_1. Considering the traction β_1 in the direction $i = 1$, the other elements of the deformation gradient are

$$\beta_2 = \beta_3 = \beta_1^{-1/2} \,. \tag{32}$$

The Cauchy stress of the simple traction is given as

$$\sigma = \beta_1 \frac{\mathrm{d}W}{\mathrm{d}\beta_1} \,, \tag{33}$$

where W is a strain-energy function. Using again the definitions (13) and (21), the corresponding stresses σ_{BS} (exact) and σ_{bs} (approximate) are determined. The resulting stress-strain characteristics are depicted in the figure 4. On the left side, two limit cases $P_1 = 0$ and $P_1 = 1$ representing the material with no prestress and with the maximum prestress are chosen. The influence of the prestress is clearly shown by stiffening the material. The curves corresponding to σ_{BS} and σ_{bs} differ since the material parameters are chosen such that the accuracy conditions (24) do not hold. On the right side, several curves representing the different values of prestress are depicted. The accuracy conditions are fulfilled, so the curves representing σ_{BS} and σ_{bs} coincide. Again, the material gets stiffer with the increasing prestress demonstrating the influence of the micro-parameter on the macro-behaviour. Notice that the tangents of the curves in the origin differ expressing the different Young's moduli according to (29).

6. Conclusion

In this paper, a two-scale hyperelastic model of a soft tissue is proposed which includes the prestress at the reference state. At the micro-level, a simple mechanical model of a living cell with surrounding extracellular matrix is created using linear elastic elements. Due to the assumption of the cell constant volume, the pre-existing tension is maintained within the microstructure with no additional struts. The influence of the prestress on the mechanical response of the

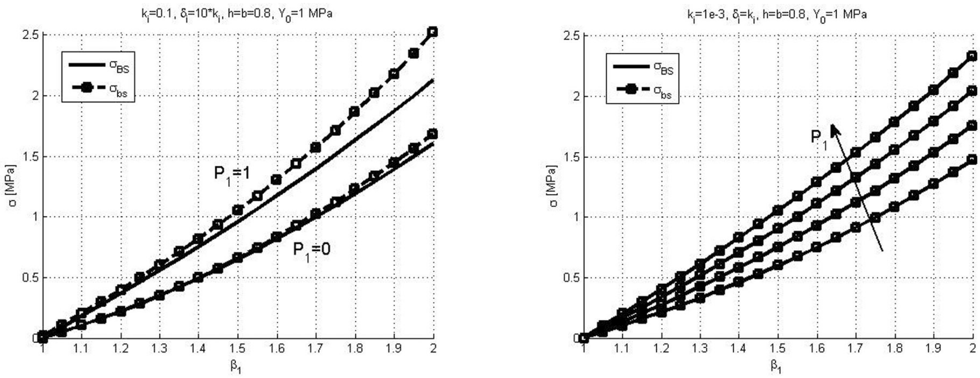

Fig. 4. Stress-strain characteristics. Comparison between σ_{BS} and σ_{bs} (left). The dependence of the stress-strain macroscopic behaviour on the prestress (right)

microstructure is shown by deriving the formula of the Young's modulus. It exhibits a clear dependence on prestress, the so-called prestress-induced stiffening, that is observed for living cells. In our proposed model, the stiffness of the cell is doubled by prestress in the limit case.

In the continuum limit, the mechanical model of a living cell is considered as a single material point at the macro-scale. Thus the hyperelastic model of a soft tissue is developed taking into account the arrangement of microstructure. Although there is no analytical expression of the strain-energy function, an approximation is found which is suitable for soft tissues (e.g. for smooth muscles). Although based on the linear elastic elements, the behaviour of the model is highly nonlinear due to the incompressibility assumptions at the both micro- and macro-level. This is shown on a simple traction test, for which the model exhibits the strain-hardening. Such behaviour, i.e. the increasing stiffness with the increasing deformation, is experimentally observed for soft tissues.

The traction test also shows the influence of the prestress on the macroscopic behaviour. With the increasing prestress, the stiffness of the material increases for any strain. It means that the present model predicts the prestress-induced stiffening also at the macro-scale, i.e. at the tissular level. Such feature has not been widely studied, so there is a lack of experimental observations. Therefore, we cannot compare our results with experimental data in the present paper. However, the results are promising for further studies of processes within soft tissues involving the prestress. In fact, the model allows to control the macroscopic response by setting the parameter at the micro-scale. Concretely, by changing the rest length of the fibres within the living cells (setting the prestress), the overall response is either softer or stiffer. This can be used e.g. for studying of some aspects of muscle contraction which is accompanied by changing the rest lengths of fibres within muscle cells.

We are aware that the proposed model cannot be capable of describing living tissues in full complexity. The aim of the present work is not to propose a realistic model of living tissues but to emphasize a certain feature, the prestress. The aim for the future is to extend the present model so that it is possible to consider a general deformation, not only the special case described by diagonal deformation gradient.

Acknowledgements

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