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# Passive and active fibre reorientation in anisotropic materials

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## Abstract

We present a continuum model to describe the reorientation of an anisotropic material structure, characterized by two fiber families able to modify their orientations following different evolution dynamics. The evolution equations are derived in a thermodynamically consistent way, and passive and active contributions to the reorientation process are identified. It is shown that a weaker extension of a well-known coaxiality result holds. The transversely isotropic and orthotropic cases are then recovered by imposing the proper constraint on the fiber rotation. Applications to biological experiments on cell layers under stretch are discussed, showing a good agreement between the model and the experimental results. Even though we focus on cell layers, our framework remains general and may be employed to describe reorientation in engineering materials.

**Keywords:** Fibre reorientation · Anisotropic materials · Nonlinear elasticity · Coaxiality · Cell orientation · Stress fibers

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## Conflict of interest statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Abstract

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## 1. Introduction

2     The ability of actively changing the internal structure in response to ex-  
3     ternal stimuli is a fundamental characteristic of biological tissues, cells, and  
4     organisms. Such a process, which is generally referred to as *remodeling*, may  
5     be driven by growth, injuries, ageing or alterations in the chemo-mechanical  
6     environment, to cite but a few examples [1, 2, 3, 4, 5]. As a consequence  
7     of these prompts, a reorganization of the biological microstructure is often  
8     observed, since the material constantly tries to adapt to the new conditions  
9     in a dynamic way. Understanding and accurately describing the remodeling  
10    of living structures is a major challenge in biomechanics, which has been of  
11    great interest in recent years: from a mechanical viewpoint, several works  
12    have focused on different features of remodeling, such as the coupling with  
13    growth [4, 6, 7], the influence of diseases in shape alterations [8] or in ma-  
14    terial properties, and the changes in the biological structure as plastic-like

1 irreversible distortions [9]; see also [10] and references therein for a detailed  
2 overview of remodeling and growth in soft tissues.

3 Among the several types of remodeling that may be triggered by external  
4 forces, reorientation is probably one of the most relevant as far as living  
5 tissues and matter are concerned. For a biological material with a fiber-  
6 reinforced structure, it can be defined as a change in the local orientation  
7 of fibers due to some external actions, leading therefore to a reorganization  
8 in the microstructure of the material. This phenomenon is frequently seen  
9 in different situations: for instance, it is well known that the bones are able  
10 to change the orientation of their internal fibers to functionally adapt to  
11 environmental stimuli [11]. In particular, many biological materials with a  
12 fiber-like microstructure are described as transversely isotropic, that is, a  
13 single preferential direction exists and influences the mechanical behaviour:  
14 significant examples are articular cartilage, tendons or skin, to cite but a  
15 few [7, 12, 13, 14, 15, 16]. Instead, it is worth mentioning that tissues may  
16 exhibit an orthotropic arrangement, which requires the description of two  
17 distinct fiber directions. A significant example can be found in the circu-  
18 latory system, where the myocardium and the arteries are known to have  
19 three planes with distinct mechanical properties [17, 18, 19, 20, 21]. An-  
20 other phenomenon related to orthotropy that has recently gathered some  
21 attention is the cellular response to mechanical cues coming from the sur-  
22 rounding microenvironment. In particular, experiments have demonstrated  
23 that cells seeded on a two-dimensional substrate which is cyclically stretched  
24 reorient their stress fibers and bodies to reach a stable configuration, charac-  
25 terized by a precise angle between the cell axis and the direction of stretching  
26 [22, 23, 24, 25, 26, 27, 28, 29].

27 A possible explanation of this behaviour, that relies on mechanical ar-  
28 guments, has been firstly proposed by Livne et al. [22], who suggested that  
29 cells attempt to minimize the elastic energy stored in the stretching process.  
30 Recently, a generalization of the energy considered in [22] was presented in  
31 [30, 31], where the system composed by the cells and the substrate was de-  
32 scribed as an orthotropic material: the preferential directions were identified  
33 with the cellular actin stress fibers and with the orthogonal protein network  
34 interconnecting them [32, 33, 34, 35].

35 However, the nonlinear elastic description of cell orientations proposed in  
36 [30] does not explicitly include a remodeling of the internal structure, even  
37 if the material composed by substrate and cells is treated as orthotropic.  
38 Instead, cells are viewed as passive fibers whose reorientation is dragged by  
39 the deformation of the layer itself. A different point of view, even if limited  
40 to transversely isotropic materials, has been recently proposed in [36, 37],

1 taking into account both passive and active changes in the fiber directions.  
2 The introduction of a remodeling equation, that complements the usual  
3 mechanical balances, allows to describe the evolution of fiber orientation  
4 under mechanical [36] and magnetic [37] stimuli. Moreover, in [36], it was  
5 shown that the stationary solutions of the remodeling equation are the ones  
6 that make the remodeled stress and strain tensors coaxial [38].

7 It seems then quite natural to provide an extension of the results pre-  
8 sented in [36] to a more general case, where an hyperelastic material is  
9 endowed with a double fiber microstructure, as in the cellular example.  
10 Furthermore, while in [30] the two fibers were fixed to be perpendicular,  
11 it is of interest to characterize the remodeling of the different fiber families  
12 independently, in a way that each fiber can change the orientation according  
13 to its own rotation tensor.

14

15 In this paper, motivated by these observations, we propose a mechanical  
16 model that describes the reorganization of an anisotropic material struc-  
17 ture, characterized by two fiber families that can modify their orientation  
18 following different evolution equations. Both active contributions affecting  
19 the reorientation process, like external forces or stimuli, and purely passive  
20 material remodeling can be incorporated in the proposed framework. In do-  
21 ing so, we are able to extend an energetic modeling of cell alignment [22, 30]  
22 using a fiber reorientation framework [36], in which the rotation of the cells  
23 due to the mechanical prompt is treated as an additional variable for the  
24 model. This allowed us to derive the reorientation equations in a rigorous  
25 and thermodynamically consistent basis, recovering the results presented in  
26 [30] as a particular case. At the same time, we provide an extension of the  
27 fiber reorientation model proposed in [36], adapting it to anisotropic ma-  
28 terials with two preferential directions that can change their orientation in  
29 different manners, even though they can be properly coupled. The limit of  
30 two families of fibers which cannot change their relative orientation, as done  
31 for instance by Menzel [39] in the orthotropic case, is recovered within the  
32 terms of a constrained model.

33 The paper is organized as follows. Section 2 presents the remodeling frame-  
34 work in presence of a double-fibered anisotropic internal material structure,  
35 through a generalization of the model proposed in [36]. Then, in Section  
36 3, the stationary solutions of the reorientation equations for the fibers are  
37 thoroughly studied, showing that a weaker extension of the coaxiality result  
38 by Vianello [38] holds when the fiber reinforcements are able to reorient  
39 without any constraint. Section 4 is devoted to the analysis of an in-plane  
40 situation, where the fibers are supposed to lie in a plane during the whole

1 remodeling process. In this case, we are able to specify the general evolution  
 2 equations and the related stationary solutions, focusing for simplicity on a  
 3 minimal elastic energy which however allows relevant comparisons with ex-  
 4 perimental data. Section 5 is devoted to the discussion of a reduced model  
 5 based on an orthotropic material structure with fixed relative orientation  
 6 of the fibers, naturally emerging from the general framework, provided that  
 7 a constraint on fiber rotations is included. Applications of the proposed  
 8 models in the biological context of cell orientation are then presented in  
 9 Section 6. In particular we show that, as expected, the constrained model is  
 10 consistent with some already known results, such as the phenomenological  
 11 evolution equation for cell orientation postulated by Livne et al. [22] and  
 12 the stationary points of the energy derived in [30]. Moreover, the general  
 13 model is employed to describe stress fibers and cell nucleus reorientation,  
 14 showing a [good agreement](#) with experimental data by Roshanzadeh et al.  
 15 [29]. Finally, in Section 7 we provide some discussion and conclusions, as  
 16 well as future possible developments and applications of the present theory.  
 17 Appendix A is dedicated to the discussion of another possible choice for the  
 18 constraint between the fiber families.

## 19 **2. Remodeling framework**

20 Following the approach proposed in [36], we describe the reorientation  
 21 within the general framework of finite elasticity with remodeling presented  
 22 in [40]. We consider a material equipped with an anisotropic two families  
 23 of fibers (TFF) internal structure whose change of orientation is not simply  
 24 dragged by the deformation but described by additional state variables,  
 25 therefore including a remodeling of the fiber structure. The relationship  
 26 between fiber orientations and mechanical forces, as well as the constitutive  
 27 coupling between the two fiber families which characterize the anisotropic  
 28 structure, are derived on a thermodynamically consistent basis.

### 29 *2.1. Kinematics*

30 Given a body, identified with a region  $\mathcal{B}_r$  of the Euclidean three-dimensional  
 31 space  $\mathcal{E}$ , and a material point  $X \in \mathcal{B}_r$ , we consider the time-dependent  
 32 map  $\chi : \mathcal{B}_r \times \mathcal{T} \rightarrow \mathcal{E}$ , called the deformation<sup>1</sup> of the body, that assigns  
 33 to each point  $X \in \mathcal{B}_r$  a point  $x = \chi(X, t)$  at any instant  $t$  of the time  
 34 interval  $\mathcal{T}$  and determines the current configuration  $\mathcal{B} = \chi(\mathcal{B}_r, t)$  of the

---

<sup>1</sup>We consider deformations that are twice continuously differentiable.

1 body at time  $t$ . As standard in finite elasticity, we introduce the displace-  
 2 ment field  $\mathbf{u} : \mathcal{B}_r \times \mathcal{T} \rightarrow \mathcal{V}$ , with  $\mathcal{V}$  the translation space of  $\mathcal{E}$ , such that  
 3  $x = \chi(X, t) = X + \mathbf{u}(X, t)$ , and the fields

$$\mathbf{F}(X, t) = \nabla \chi(X, t) \quad \text{and} \quad \dot{\chi}(X, t) = \frac{\partial \chi}{\partial t}(X, t), \quad (2.1)$$

4 that represent the deformation gradient and the material velocity field, re-  
 5 spectively. Clearly,  $\mathbf{F} = \mathbf{I} + \nabla \mathbf{u}$ , where  $\mathbf{I}$  is the identity tensor. We assume  
 6 that at a certain time instant  $t = t_0$ , the body occupies the reference con-  
 7 figuration, that is,  $\chi(X, t_0) = X$  for each point in  $\mathcal{B}_r$  and  $\mathbf{u}(X, t_0) = \mathbf{0}$ .  
 8 In addition to the displacement field describing the current position of the  
 9 body, we are interested in the evolution of the orientation of the anisotropic  
 10 TFF internal structure, which in  $\mathcal{B}_r$  is based on the pair of material unit  
 11 vector fields  $\mathbf{a}_0 : \mathcal{B}_r \rightarrow \mathcal{V}$  and  $\mathbf{b}_0 : \mathcal{B}_r \rightarrow \mathcal{V}$  (with  $|\mathbf{a}_0| = |\mathbf{b}_0| = 1$ ); they  
 12 represent the preferred directions that the internal structure endows to the  
 13 material, i.e. the direction of each fiber at  $X \in \mathcal{B}_r$ . For practical usage, it  
 14 is convenient to introduce the corresponding *structural or orientation ten-*  
 15 *sors*<sup>2</sup> at  $\mathcal{B}_r$ , defined as  $\mathbf{A}_0 = \mathbf{a}_0 \otimes \mathbf{a}_0$  and  $\mathbf{B}_0 = \mathbf{b}_0 \otimes \mathbf{b}_0$ . In the following,  
 16 we will sometimes refer to the field  $\mathbf{a}_0$  as the *primary structure* of the ma-  
 17 terial, while  $\mathbf{b}_0$  will be consequently called *secondary structure*. Both  $\mathbf{A}_0$   
 18 and  $\mathbf{B}_0$  contribute to the material anisotropy and can reorient as prescribed  
 19 by two different rotation fields, each one interpreted as the rotation of a  
 20 single fiber family. In this respect, we will consider a time-dependent tensor  
 21 field  $\mathbf{R}_p : \mathcal{B}_r \times \mathcal{T} \rightarrow \mathbb{R}\text{ot}$  which represents the reorientation of the primary  
 22 structure and changes the reference orientation from  $\mathbf{a}_0(X)$  to

$$\mathbf{a}(X, t) = \mathbf{R}_p(X, t)\mathbf{a}_0(X),$$

23 or equivalently  $\mathbf{A}_0(X)$  to

$$\mathbf{A}(X, t) = \mathbf{R}_p(X, t)\mathbf{A}_0(X)\mathbf{R}_p^T(X, t), \quad (2.2)$$

24 where  $\mathbf{A} = \mathbf{a} \otimes \mathbf{a}$ . Likewise, the second rotation field  $\mathbf{R}_s : \mathcal{B}_r \times \mathcal{T} \rightarrow \mathbb{R}\text{ot}$   
 25 describes the reorientation of the secondary structure and changes  $\mathbf{b}_0(X)$  to

$$\mathbf{b}(X, t) = \mathbf{R}_s(X, t)\mathbf{b}_0(X)$$

26 and  $\mathbf{B}_0(X)$  to

$$\mathbf{B}(X, t) = \mathbf{R}_s(X, t)\mathbf{B}_0(X)\mathbf{R}_s(X, t)^T, \quad (2.3)$$

---

<sup>2</sup>Typically, they are denoted *structural tensors* in the mechanics of fiber-reinforced materials [18] and *orientation tensors* in the literature on nematic liquid crystals [41].

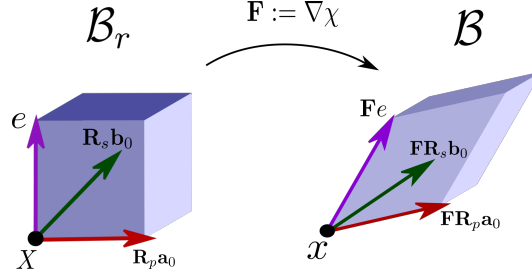


Figure 1: Schematic representation of the reorientation process at a material point. A material line element  $e$  in the reference configuration  $\mathcal{B}_r$  is deformed to the corresponding line element  $\mathbf{F}e$  in the current configuration  $\mathcal{B}$ . Instead, the primary structure  $\mathbf{a}_0$  firstly undergoes remodeling due to the rotation  $\mathbf{R}_p$  while the secondary structure  $\mathbf{b}_0$  is reoriented according to another rotation  $\mathbf{R}_s$ .

1 having denoted  $\mathbf{B} = \mathbf{b} \otimes \mathbf{b}$ . Each fiber family of such an anisotropic material  
 2 may change its orientation as time evolves; then, the deformation gradient  
 3 tensor  $\mathbf{F}$  maps each remodeled fiber to the current configuration, as sketched  
 4 in Fig. 1. With these definitions on hand, the state variables of the problem  
 5 are the displacement and rotation fields, that is, the triple  $(\mathbf{u}, \mathbf{R}_p, \mathbf{R}_s) \in$   
 6  $\mathcal{V} \times \text{Rot} \times \text{Rot}$ , and the corresponding velocity fields are identified by the  
 7 time derivatives  $(\dot{\mathbf{u}}, \dot{\mathbf{R}}_p \mathbf{R}_p^T, \dot{\mathbf{R}}_s \mathbf{R}_s^T) \in \mathcal{V} \times \text{Skw} \times \text{Skw}$ , where  $\text{Skw}$  denotes  
 8 the space of skew-symmetric tensors. Finally, we denote as  $(\mathbf{w}, \mathbf{W}_p, \mathbf{W}_s) \in$   
 9  $\mathcal{V} \times \text{Skw} \times \text{Skw}$  the associated virtual velocity fields.

10 *Remark.* Let us note that our kinematic framework does not filter out the  
 11 rotation fields  $\mathbf{R}_p$  and  $\mathbf{R}_s$  such that  $\mathbf{R}_p \mathbf{a}_0 = \mathbf{a}_0$  and  $\mathbf{R}_s \mathbf{b}_0 = \mathbf{b}_0$ , which are  
 12 included in the admissible rotation fields even if they maintain the energy  
 13 unchanged and so are of no interest in the remodeling problem.

## 14 2.2. Balance equations

15 The balance equations of the model are delivered by the principle of  
 16 virtual working, based on the choice of the external and internal virtual  
 17 workings defined as continuous, linear, real-valued functionals on the space  
 18 of virtual velocities. By introducing forces and torques of the model which  
 19 are working-conjugate to each kinematic variable, we write

$$\mathcal{W}_e(\mathbf{w}, \mathbf{W}_p, \mathbf{W}_s) = \int_{\mathcal{B}_r} (\mathbf{z} \cdot \mathbf{w} + \mathbf{Z}_p \cdot \mathbf{W}_p + \mathbf{Z}_s \cdot \mathbf{W}_s) dV + \int_{\partial_t \mathcal{B}_r} \mathbf{s} \cdot \mathbf{w} dA \quad (2.4)$$

20 for the external virtual working and

$$\mathcal{W}_i(\mathbf{w}, \mathbf{W}_p, \mathbf{W}_s) = \int_{\mathcal{B}_r} (\mathbf{S} \cdot \nabla \mathbf{w} + \Sigma_p \cdot \mathbf{W}_p + \Sigma_s \cdot \mathbf{W}_s) dV \quad (2.5)$$



1 for the internal virtual working. The pair  $(\mathbf{z}, \mathbf{s})$  are forces per unit of (ref-  
2 erential) volume and area, respectively, while  $\mathbf{S}$  is the first Piola–Kirchhoff  
3 stress tensor. The pair of skew tensors  $(\mathbf{Z}_i, \mathbf{\Sigma}_i)$ , with  $i = p, s$ , are torques  
4 per unit of (referential) volume, and represent the outer and inner remodel-  
5 ing torques, as  $\mathbf{W}_p, \mathbf{W}_s$  are skew-symmetric tensors. More specifically, the  
6 outer torques  $\mathbf{Z}_p$  and  $\mathbf{Z}_s$  represent external source terms which may affect  
7 fiber reorientation, for instance magnetic effects [37] or chemo-mechanical  
8 processes. On the other side, the inner remodeling torques  $\mathbf{\Sigma}_p$  and  $\mathbf{\Sigma}_s$  take  
9 into account the internal actions driving the reorientation of the primary  
10 and secondary material structures, respectively. It is worth remarking that,  
11 for what concerns the remodeling torques, our theory is of order zero-th,  
12 i.e., we do not take into account the gradients of the rotation fields, which  
13 instead may become relevant when the fibers are closely packed.

14 By enforcing the condition that the external and internal virtual working  
15 be equal for any virtual velocities  $(\mathbf{w}, \mathbf{W}_p, \mathbf{W}_s) \in \mathcal{V} \times \text{Skw} \times \text{Skw}$  and for any  
16 subregion  $\mathcal{R} \subset \mathcal{B}_r$ , we obtain the following balance equations and associated  
17 boundary conditions:

$$\text{Div } \mathbf{S} + \mathbf{z} = \mathbf{0} \quad \text{and} \quad \mathbf{\Sigma}_p = \mathbf{Z}_p \quad \text{and} \quad \mathbf{\Sigma}_s = \mathbf{Z}_s \quad \text{in } \mathcal{B}_r, \quad (2.6)$$

$$18 \quad \mathbf{u} = \hat{\mathbf{u}} \quad \text{on } \partial_u \mathcal{B}_r \quad \text{and} \quad \mathbf{S} \mathbf{m} = \mathbf{s} \quad \text{on } \partial_t \mathcal{B}_r, \quad (2.7)$$

19 with  $\partial_u \mathcal{B}_r$  and  $\partial_t \mathcal{B}_r$  denoting parts of the boundary  $\partial \mathcal{B}_r$  where displacements  
20 and tractions are respectively prescribed, and  $\mathbf{m}$  denoting the unit normal  
21 to  $\partial_t \mathcal{B}_r$ . Equations (2.6) are the three balance equations of our theory. The  
22 first is the usual balance of mechanical forces, where inertial effects can be  
23 included in the bulk force  $\mathbf{z}$ , even if in the present model they are neglected  
24 since the remodeling time scale is typically much longer than the inertial  
25 one. The second and third equations are the balances of the remodeling  
26 torques, driving the reorientation of the primary and secondary structures,  
27 respectively, once the appropriate constitutive equations will be considered.  
28 In particular, they prescribe that the outer and inner remodeling torques be  
29 equal. These equations generalise the theory presented in [36], where only  
30 a transversely isotropic internal structure was considered.

31 The external working, that corresponds to balanced forces and torques and  
32 is evaluated on the actual velocity fields  $(\dot{\mathbf{u}}, \dot{\mathbf{R}}_p \mathbf{R}_p^T, \dot{\mathbf{R}}_s \mathbf{R}_s^T)$ , identifies the  
33 external actual power  $\mathcal{P}_e$  expended during the evolution of the continuum:

$$\begin{aligned} \mathcal{W}_e(\dot{\mathbf{u}}, \dot{\mathbf{R}}_p \mathbf{R}_p^T, \dot{\mathbf{R}}_s \mathbf{R}_s^T) &= \int_{\mathcal{B}_r} (\mathbf{z} \cdot \dot{\mathbf{u}} + \mathbf{Z}_p \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T + \mathbf{Z}_s \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T) dV + \int_{\partial_t \mathcal{B}_r} \mathbf{s} \cdot \dot{\mathbf{u}} dA \\ &= \int_{\mathcal{B}_r} (\mathbf{S} \cdot \dot{\mathbf{F}} + \mathbf{\Sigma}_p \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T + \mathbf{\Sigma}_s \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T) = \mathcal{P}_e. \end{aligned} \quad (2.8)$$

1 *2.3. Constitutive equations and energy imbalance*

2 The constitutive recipes to describe the behaviour of the material with  
 3 the reorientable anisotropic TFF internal structure are prescribed in a ther-  
 4 modynamically consistent way, through the following steps. Firstly, we take  
 5 into account a class of materials that admits an elastic strain energy density  
 6 in the form

$$\varphi = \phi(\mathbf{E}, \mathbf{A}, \mathbf{B}) = \psi(\mathbf{E}, \mathbf{R}_p, \mathbf{R}_s), \quad (2.9)$$

7 dependent upon the deformation  $\mathbf{F}$  through the Green–Lagrange strain ten-  
 8 sor  $\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$ , and on the remodeled orientation tensors  $\mathbf{A}$  and  $\mathbf{B}$   
 9 or, equivalently, on the rotations  $\mathbf{R}_p$  and  $\mathbf{R}_s$  that transform the primary  
 10 and secondary structures. More specifically, following the theory of double-  
 11 fibered finite elasticity, we assume that  $\phi$  and  $\psi$  are isotropic functions of  
 12 their arguments [42, 43].

13 We also assume that dissipation is only associated with the remodeling  
 14 processes, and the dissipation density  $\delta$  can be written as

$$\delta = \delta(\dot{\mathbf{R}}_p\mathbf{R}_p^T, \dot{\mathbf{R}}_s\mathbf{R}_s^T). \quad (2.10)$$

15 To derive constitutive equations that are consistent with the first and second  
 16 laws of thermodynamics, we enforce the energy imbalance, stating that for  
 17 any admissible process, characterised by the state variables  $(\mathbf{u}, \mathbf{R}_p, \mathbf{R}_s)$ , the  
 18 time derivative of the energy must not exceed the external actual power  
 19 expended on the body along the same process, i.e., the dissipation must be  
 20 positive:

$$\int_{\mathcal{B}_r} \delta dV = \mathcal{P}_e - \int_{\mathcal{B}_r} \dot{\varphi} dV \geq 0. \quad (2.11)$$

21 Within the framework discussed so far and using Eq. (2.9), we can write the  
 22 time derivative of the elastic energy as

$$\dot{\varphi} = \frac{\partial\phi}{\partial\mathbf{E}} \cdot \dot{\mathbf{E}} + \frac{\partial\phi}{\partial\mathbf{A}} \cdot \dot{\mathbf{A}} + \frac{\partial\phi}{\partial\mathbf{B}} \cdot \dot{\mathbf{B}}. \quad (2.12)$$

At this point, it is useful to introduce the commutator operator between  
 two tensors  $[\cdot, \cdot] : \mathbb{Lin} \times \mathbb{Lin} \rightarrow \mathbb{Lin}$ , where  $\mathbb{Lin}$  stands for the space of  
 second-order tensors, defined as:

$$[\mathbf{X}, \mathbf{Y}] = \mathbf{X}\mathbf{Y} - \mathbf{Y}\mathbf{X}, \quad \forall \mathbf{X}, \mathbf{Y} \in \mathbb{Lin}.$$

23 With this definition on hand, recalling Eqs. (2.2)-(2.3) we have

$$\dot{\mathbf{A}} = [\dot{\mathbf{R}}_p\mathbf{R}_p^T, \mathbf{A}] \quad \text{and} \quad \dot{\mathbf{B}} = [\dot{\mathbf{R}}_s\mathbf{R}_s^T, \mathbf{B}], \quad (2.13)$$

and, in general, for any  $\mathbf{X}, \mathbf{Y} \in \mathbb{L}\text{in}$ ,

$$\mathbf{X} \cdot [\dot{\mathbf{R}}_p \mathbf{R}_p^T, \mathbf{A}] = \dot{\mathbf{R}}_p \mathbf{R}_p^T \cdot [\mathbf{X}, \mathbf{A}] \quad \text{and} \quad \mathbf{Y} \cdot [\dot{\mathbf{R}}_s \mathbf{R}_s^T, \mathbf{B}] = \dot{\mathbf{R}}_s \mathbf{R}_s^T \cdot [\mathbf{Y}, \mathbf{B}],$$

1 which allow Eq. (2.12) to be rewritten as

$$\dot{\varphi} = \frac{\partial \phi}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} + \left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T + \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T. \quad (2.14)$$

2 The constitutive prescriptions for the stress  $\mathbf{S}$  and for the inner remodeling  
 3 actions  $\Sigma_p$  and  $\Sigma_s$  have to satisfy the imbalance principle stated above,  
 4 which can be rephrased in local form requiring that

$$\delta = \mathbf{S} \cdot \dot{\mathbf{F}} + \Sigma_p \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T + \Sigma_s \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T - \dot{\varphi} \geq 0 \quad (2.15)$$

5 has to be positive for every realizable process [44]. By using equations  
 6 (2.12)-(2.14), we reduce the inequality (2.15) to:

$$\left( \mathbf{S} - \mathbf{F} \frac{\partial \phi}{\partial \mathbf{E}} \right) \cdot \dot{\mathbf{F}} + \left( \Sigma_p - \left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] \right) \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T + \left( \Sigma_s - \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] \right) \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T \geq 0. \quad (2.16)$$

7 Since we assume that dissipation is only due to remodeling, the constitutive  
 8 equation for the stress can be chosen as a standard hyperelastic law:

$$\mathbf{S} = \mathbf{F} \frac{\partial \phi}{\partial \mathbf{E}}, \quad \mathbf{S}_c = \mathbf{F}^{-1} \mathbf{S} = \frac{\partial \phi}{\partial \mathbf{E}}, \quad (2.17)$$

where  $\mathbf{S}_c$  is the second Piola-Kirchhoff stress tensor. The remainder of the  
 dissipation inequality (2.16) can be satisfied on assuming that each inner  
 remodeling torque can be decomposed into an elastic and a dissipative part:

$$\Sigma_p = \Sigma_p^{(e)} + \Sigma_p^{(d)} = \left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] + \mathbb{D}_p \dot{\mathbf{R}}_p \mathbf{R}_p^T, \quad (2.18)$$

$$\Sigma_s = \Sigma_s^{(e)} + \Sigma_s^{(d)} = \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] + \mathbb{D}_s \dot{\mathbf{R}}_s \mathbf{R}_s^T, \quad (2.19)$$

9 where  $\mathbb{D}_p$  and  $\mathbb{D}_s$  are positive-definite fourth order tensors that represent the  
 10 resistance to remodeling of the primary and secondary material structure,  
 11 respectively.

12 By substituting the constitutive equations (2.17)-(2.19) in the balance equa-  
 13 tions (2.6), we are able to obtain two differential equations that describe the  
 14 evolution of the rotation fields, and therefore of the associated fiber families.  
 15 The general remodeling problem for the anisotropic TFF microstructure can

1 then be expressed as the following system of nonlinear ordinary differential  
 2 equations in  $\mathcal{B}_r \times \mathcal{T}$ :

$$\begin{cases} \mathbb{D}_p \dot{\mathbf{R}}_p \mathbf{R}_p^T = \mathbf{Z}_p - [\frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A}], \\ \mathbb{D}_s \dot{\mathbf{R}}_s \mathbf{R}_s^T = \mathbf{Z}_s - [\frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B}], \end{cases} \quad (2.20)$$

3 with initial conditions

$$\mathbf{R}_p = \mathbf{I} \quad \text{and} \quad \mathbf{R}_s = \mathbf{I} \quad \text{in} \quad \mathcal{B}_r \times \{t_0\}. \quad (2.21)$$

4 The problem (2.20) has to be solved together with the balance of forces (2.6)<sub>1</sub>  
 5 and the constitutive prescription (2.17). We observe that the elastic terms on  
 6 the right-hand side of Eqs. (2.20), represented by the commutators, include  
 7 the mutual interaction between the two fiber families, as it will be explicitly  
 8 shown in the case of plane remodeling. Moreover, when  $\mathbf{Z}_p = \mathbf{Z}_s = \mathbf{0}$ , as we  
 9 shall assume in the rest of the paper, the stationary solutions of the system  
 10 (2.20) are determined by solving the equations

$$[\frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A}] = \mathbf{0} \quad \text{and} \quad [\frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B}] = \mathbf{0}. \quad (2.22)$$

#### 11 2.4. Further constitutive prescriptions

12 For the calculations carried out in the following Sections, it is convenient  
 13 to express the strain energy density in terms of the invariants of the tensors  
 14  $\mathbf{E}$ ,  $\mathbf{A}$  and  $\mathbf{B}$ . In doing so we introduce the following classical set of isotropic  
 15 invariants of  $\mathbf{E}$ :

$$\mathbf{J}_1 = \mathbf{E} \cdot \mathbf{I}, \quad \mathbf{J}_2 = \mathbf{E}^\dagger \cdot \mathbf{I}, \quad \mathbf{J}_3 = \det(\mathbf{I} + 2\mathbf{E}), \quad (2.23)$$

16 where  $\mathbf{E}^\dagger = (\det \mathbf{E})\mathbf{E}^{-T}$ , together with the anisotropic ones [45]

$$\begin{aligned} \mathbf{J}_4 &= \mathbf{E} \cdot \mathbf{A}, & \mathbf{J}_5 &= \mathbf{E}^2 \cdot \mathbf{A}, \\ \mathbf{J}_6 &= \mathbf{E} \cdot \mathbf{B}, & \mathbf{J}_7 &= \mathbf{E}^2 \cdot \mathbf{B}, \\ \mathbf{J}_8 &= \mathbf{E} \cdot \text{sym}(\mathbf{A}\mathbf{B}) = (\mathbf{a} \cdot \mathbf{b})(\mathbf{E}\mathbf{a} \cdot \mathbf{b}). \end{aligned} \quad (2.24)$$

17 The anisotropic invariants  $\mathbf{J}_4$  and  $\mathbf{J}_6$  take into account the deformations  
 18 along the directions of the primary and secondary internal structures, while  
 19  $\mathbf{J}_5$  and  $\mathbf{J}_7$  are also measures of fiber stretch but include the influence of shear  
 20 on the fibers [46];  $\mathbf{J}_8$  is instead used to account for the interactions between

1 the two fiber families.<sup>3</sup> If we use the representation theorem for isotropic  
 2 scalar functions of three symmetric tensors (see [47, 48, 49]), we can write

$$\varphi = \phi(\mathbf{E}, \mathbf{A}, \mathbf{B}) = \hat{\phi}(J_1, J_2, J_3, J_4, J_5, J_6, J_7, J_8). \quad (2.25)$$

3 On adopting the representation (2.25) and denoting with  $\hat{\phi}_i := \partial\hat{\phi}/\partial J_i$ ,  
 4  $i = 1, \dots, 8$ , one has:

$$\begin{aligned} \frac{\partial\phi}{\partial\mathbf{E}} &= \hat{\phi}_1\mathbf{I} + \hat{\phi}_2(J_1\mathbf{I} - \mathbf{E}) + 2\hat{\phi}_3J_3(2\mathbf{E} + \mathbf{I})^{-1} + \hat{\phi}_4\mathbf{A} + \hat{\phi}_5(\mathbf{AE} + \mathbf{EA}), \\ &+ \hat{\phi}_6\mathbf{B} + \hat{\phi}_7(\mathbf{BE} + \mathbf{EB}) + \frac{1}{2}\hat{\phi}_8(\mathbf{AB} + \mathbf{BA}), \end{aligned} \quad (2.26)$$

$$\frac{\partial\phi}{\partial\mathbf{A}} = \hat{\phi}_4\mathbf{E} + \hat{\phi}_5\mathbf{E}^2 + \frac{1}{2}\hat{\phi}_8(\mathbf{EB} + \mathbf{BE}), \quad (2.27)$$

$$\frac{\partial\phi}{\partial\mathbf{B}} = \hat{\phi}_6\mathbf{E} + \hat{\phi}_7\mathbf{E}^2 + \frac{1}{2}\hat{\phi}_8(\mathbf{EA} + \mathbf{AE}). \quad (2.28)$$

5 In the following, for the sake of a lighter notation, we will drop the hat from  
 6 the derivatives of the strain energy with respect to the invariants.

7 *Remark.* It is often customary to express  $\hat{\phi}$  in terms of the invariants of the  
 8 right Cauchy–Green strain tensor  $\mathbf{C} = \mathbf{F}^T\mathbf{F}$  rather than  $\mathbf{E}$ :

$$\begin{aligned} I_1 &= \mathbf{C} \cdot \mathbf{I}, & I_2 &= \mathbf{C}^\dagger \cdot \mathbf{I}, & I_3 &= \det \mathbf{C}, \\ I_4 &= \mathbf{C} \cdot \mathbf{A}, & I_5 &= \mathbf{C}^2 \cdot \mathbf{A}, \\ I_6 &= \mathbf{C} \cdot \mathbf{B}, & I_7 &= \mathbf{C}^2 \cdot \mathbf{B}, \\ I_8 &= \mathbf{C} \cdot \text{sym}(\mathbf{AB}). \end{aligned} \quad (2.29)$$

However, since the relationship  $\mathbf{C} = 2\mathbf{E} + \mathbf{I}$  holds true, the two sets of

---

<sup>3</sup>The coupling invariant  $J_8$  may be defined in different ways. The definition of  $J_8$  in (2.24) is the one proposed in [45]; however, there are other definitions that are sometimes used in the literature. In [18], for instance, the authors use  $J_8 = \mathbf{a} \cdot \mathbf{Eb}$ . In this paper we choose the former definition, which keeps the energy invariant under change of sign of either  $\mathbf{a}$  or  $\mathbf{b}$ .

invariants are connected by the following transformations:

$$\begin{aligned}
J_1 &= \frac{1}{2}(\mathbf{I}_1 - 3), & J_2 &= \frac{1}{4}(\mathbf{I}_2 - 3) - \frac{1}{2}(\mathbf{I}_1 - 3), & J_3 &= \mathbf{I}_3, \\
J_4 &= \frac{1}{2}(\mathbf{I}_4 - 1), & J_5 &= \frac{1}{4}(\mathbf{I}_5 - 1) - \frac{1}{2}(\mathbf{I}_4 - 1), \\
J_6 &= \frac{1}{2}(\mathbf{I}_6 - 1), & J_7 &= \frac{1}{4}(\mathbf{I}_7 - 1) - \frac{1}{2}(\mathbf{I}_6 - 1), \\
J_8 &= \frac{1}{2}(\mathbf{I}_8 - \mathbf{A} \cdot \mathbf{B}).
\end{aligned} \tag{2.30}$$

### 1 3. Characterization of the remodeling stationary solutions

2 In [36], it was proved that, for materials equipped with a reorientable  
3 transversely isotropic internal structure described by a rotation field  $\mathbf{R}$  and  
4 in absence of external stimuli, the stationary solutions of the remodeling  
5 equations are those rotations which make stress  $\mathbf{S}_c$  and strain  $\mathbf{E}$ , or equiva-  
6 lently  $\mathbf{C}$ , coaxial. In addition, those rotations render the map

$$\sigma : \text{Rot} \ni \mathbf{R} \mapsto \sigma(\mathbf{R}) = \psi(\mathbf{C}, \mathbf{R})$$

7 stationary, where  $\psi(\mathbf{C}, \mathbf{R})$  is the elastic strain energy (see Proposition 1 of  
8 [36] and also [38]).

9 In this Section, it is shown that these results can be partially extended to  
10 include the anisotropic double-fibered internal structure considered here. To  
11 do so, we first note that the results in [38], often referred to as *Vianello's*  
12 *coaxiality theorem*, hold true whatever class of material symmetry is con-  
13 sidered, either isotropic or orthotropic, granted that all fiber families are  
14 transformed under the same rotation acting on the body. It is then rea-  
15 sonable to expect that, under our more general framework in which two  
16 rotations appear, there could be a loss of equivalence between coaxiality  
17 and stationarity of the energy, as we shall prove in the following.

#### 18 3.1. Stationarity and coaxiality

19 Before passing to the main result of this Section, we recall that two  
20 symmetric tensors  $\mathbf{U}, \mathbf{V}$  are said to be coaxial if they commute, or equiv-  
21 alently if their commutator vanishes, i.e.  $[\mathbf{U}, \mathbf{V}] = \mathbf{0}$ . Moreover, we prove  
22 the following relation:

$$\left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] + \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] = [\mathbf{E}, \mathbf{S}_c]. \tag{3.31}$$

By recalling (2.27) and (2.28), the left-hand side of (3.31) can be written as

$$\begin{aligned}
\left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right] + \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right] &= \phi_4[\mathbf{E}, \mathbf{A}] + \phi_5[\mathbf{E}^2, \mathbf{A}] + \phi_6[\mathbf{E}, \mathbf{B}] + \phi_7[\mathbf{E}^2, \mathbf{B}] \\
&+ \frac{\phi_8}{2}(\mathbf{EBA} + \mathbf{BEA} - \mathbf{AEB} - \mathbf{ABE}) \\
&+ \frac{\phi_8}{2}(\mathbf{EAB} + \mathbf{AEB} - \mathbf{BEA} - \mathbf{BAE}) \\
&= \phi_4[\mathbf{E}, \mathbf{A}] + \phi_5[\mathbf{E}^2, \mathbf{A}] + \phi_6[\mathbf{E}, \mathbf{B}] + \phi_7[\mathbf{E}^2, \mathbf{B}] \\
&+ \frac{\phi_8}{2}\mathbf{E}(\mathbf{BA} + \mathbf{AB}) - \frac{\phi_8}{2}(\mathbf{AB} + \mathbf{BA})\mathbf{E} \\
&= \phi_4[\mathbf{E}, \mathbf{A}] + \phi_5[\mathbf{E}^2, \mathbf{A}] + \phi_6[\mathbf{E}, \mathbf{B}] + \phi_7[\mathbf{E}^2, \mathbf{B}] + \phi_8[\mathbf{E}, \text{sym}(\mathbf{AB})]
\end{aligned}$$

which, in view of (2.26) and (2.17), is indeed equivalent to

$$\phi_4[\mathbf{E}, \mathbf{A}] + \phi_5[\mathbf{E}, \mathbf{AE} + \mathbf{EA}] + \phi_6[\mathbf{E}, \mathbf{B}] + \phi_7[\mathbf{E}, \mathbf{BE} + \mathbf{EB}] + \phi_8[\mathbf{E}, \text{sym}(\mathbf{AB})] = [\mathbf{E}, \mathbf{S}_c],$$

1 which proves Eq. (3.31). Then, at stationarity, since both the commutators  
2 on the left-hand side of (3.31) vanish,  $[\mathbf{E}, \mathbf{S}_c] = \mathbf{0}$  holds, that is, the sta-  
3 tionary solutions of (2.20) in the passive case are rotations  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  which  
4 make stress and strain coaxial. This result generalizes the one derived in  
5 [36] for transversely isotropic materials. We note however that the inverse  
6 statement is not necessarily true: in fact, coaxiality of stress and strain does  
7 not imply that both commutators have to vanish, and therefore need not be  
8 equivalent to a stationary solution of the remodeling system.

9 Taking into account this observations, we are now in the position of  
10 proving the following result <sup>4</sup>.

11 **Proposition 1.** *Let  $\mathbf{E}$  be a given deformation.*

(a)  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is a stationary solution of the passive remodeling system of equations if and only if  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is a critical point of the map

$$\sigma : \mathbb{R}\text{ot} \times \mathbb{R}\text{ot} \rightarrow \mathbb{R} \tag{3.32}$$

$$(\mathbf{R}_p, \mathbf{R}_s) \mapsto \sigma(\mathbf{R}_p, \mathbf{R}_s) = \phi(\mathbf{E}, \mathbf{A}, \mathbf{B}) = \phi(\mathbf{E}, \mathbf{R}_p \mathbf{A}_0 \mathbf{R}_p^T, \mathbf{R}_s \mathbf{B}_0 \mathbf{R}_s^T),$$

12 where  $\phi$  is the strain energy density.

---

<sup>4</sup>Proposition 1 is formulated in terms of the Green–Lagrange strain tensor  $\mathbf{E}$ . However, since the principal directions of  $\mathbf{E}$  and  $\mathbf{C}$  coincide, it could be equivalently stated in terms of the right Cauchy–Green strain tensor  $\mathbf{C}$  as was done in [36].

1 (b) If  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is a stationary solution of the remodelling system of equa-  
 2 tions, then the stress  $\mathbf{S}_c^* = \mathcal{S}(\mathbf{E}, \mathbf{R}_p^*, \mathbf{R}_s^*)$  and strain  $\mathbf{E}$  tensors are  
 3 coaxial.

*Proof.* Statement (b) follows from the discussion carried out at the beginning of this Subsection. As a matter of fact, if  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is a stationary solution of the passive remodelling system (2.20), then

$$\left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^* = \mathbf{0} \quad \text{and} \quad \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right]^* = \mathbf{0},$$

where we have used a superscript  $*$  to denote quantities at stationarity. Consequently, by (3.31),

$$\mathbf{0} = \left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^* + \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right]^* = [\mathbf{E}, \mathbf{S}_c^*]$$

4 and therefore the stress and strain tensors are coaxial. To prove statement  
 5 (a), we follow the procedure put forward by Vianello [38]. In this case,  
 6 however, we need to exploit the canonical isomorphism between the tangent  
 7 space  $\text{Rot}(\mathbf{R}_p, \mathbf{R}_s)$  to the product manifold  $\mathbb{R}\text{ot} \times \mathbb{R}\text{ot}$  at  $(\mathbf{R}_p, \mathbf{R}_s)$  and the  
 8 product space  $\text{Skw} \times \text{Skw}$ , for which

$$\text{Rot}(\mathbf{R}_p, \mathbf{R}_s) = \{(\mathbf{W}_p \mathbf{R}_p, \mathbf{W}_s \mathbf{R}_s) \mid (\mathbf{W}_p, \mathbf{W}_s) \in \text{Skw} \times \text{Skw}\}.$$

In such a case, the derivative of the energy at  $(\mathbf{R}_p, \mathbf{R}_s)$  in the direction  $(\mathbf{W}_p \mathbf{R}_p, \mathbf{W}_s \mathbf{R}_s)$  becomes

$$\begin{aligned} \dot{\sigma}(\mathbf{R}_p, \mathbf{R}_s) &= D\sigma(\mathbf{R}_p, \mathbf{R}_s)[\mathbf{W}_p \mathbf{R}_p, \mathbf{W}_s \mathbf{R}_s] = \frac{\partial\phi}{\partial\mathbf{R}_p} \cdot \mathbf{W}_p \mathbf{R}_p + \frac{\partial\phi}{\partial\mathbf{R}_s} \cdot \mathbf{W}_s \mathbf{R}_s \\ &= \left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right] \cdot \mathbf{W}_p + \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right] \cdot \mathbf{W}_s, \end{aligned}$$

9 which is null for every pair  $(\mathbf{W}_p, \mathbf{W}_s) \in \text{Skw} \times \text{Skw}$  if and only if

$$\left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^* = \mathbf{0} \quad \text{and} \quad \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right]^* = \mathbf{0}, \quad (3.33)$$

10 i.e., if and only if  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is a stationary solution of the remodelling equa-  
 11 tions.  $\square$

12 Previous derivations confirm the loss of equivalence between critical  
 13 points of the energy and coaxiality of stress and strain; indeed, in this  
 14 anisotropic TFF context, stationarity is a stronger requirement than coaxial-  
 15 ity, since it requires that both commutators have to vanish. In other words,  
 16 the set of stationary solutions is a proper subset of the set of rotations that  
 17 make the stress and strain coaxial.



#### 1 4. In-plane remodeling

2 There are many situations of interest in which both fiber families are  
3 constrained to rotate in the same plane; we refer to this situation as *in-plane*  
4 *remodeling* and study it in more detail. By introducing an orthonormal  
5 basis  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$  in the vector space  $\mathcal{V}$ , we assume that fibers lie in the  
6 plane  $\{\mathbf{e}_1, \mathbf{e}_2\}$ , whereas the rotations have an axis parallel to  $\mathbf{e}_3$  ( $\mathbf{R}_p \mathbf{e}_3 =$   
7  $\mathbf{R}_s \mathbf{e}_3 = \mathbf{e}_3$ ). We also assume that the mobility tensors are both spherical and  
8 determined by two positive scalar constants  $m_p = \mu \tau_p$  and  $m_s = \mu \tau_s$ , with  
9  $m_p \neq m_s$  in general,  $\mu$  is a shear modulus and  $\tau_p, \tau_s$  are two characteristic  
10 times of the remodeling processes:

$$\mathbb{D}_p = m_p \mathbb{I} \quad \text{and} \quad \mathbb{D}_s = m_s \mathbb{I}, \quad (4.34)$$

11 with  $\mathbb{I}$  the fourth-order identity tensor with components  $\mathbb{I}_{ijkl} = \delta_{ik} \delta_{jl}$ . Tak-  
12 ing into account that  $\dot{\mathbf{a}} = \dot{\mathbf{R}}_p \mathbf{R}_p^T \mathbf{a}$  and  $\dot{\mathbf{b}} = \dot{\mathbf{R}}_s \mathbf{R}_s^T \mathbf{b}$ , the remodeling system  
13 of equations becomes

$$\begin{cases} m_p \dot{\mathbf{a}} = -[\frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A}] \mathbf{a}, \\ m_s \dot{\mathbf{b}} = -[\frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B}] \mathbf{b}. \end{cases} \quad (4.35)$$

14 On recalling Eq. (2.27)-(2.28), the previous system can be recast in the  
15 following form:

$$\begin{cases} m_p \dot{\mathbf{a}} = (\mathbf{A} - \mathbf{I})(\phi_4 \mathbf{E} \mathbf{a} + \phi_5 \mathbf{E}^2 \mathbf{a} + \frac{\phi_8}{2} \mathbf{B} \mathbf{E} \mathbf{a} + \frac{\phi_8}{2} \mathbf{E} \mathbf{B} \mathbf{a}), \\ m_s \dot{\mathbf{b}} = (\mathbf{B} - \mathbf{I})(\phi_6 \mathbf{E} \mathbf{b} + \phi_7 \mathbf{E}^2 \mathbf{b} + \frac{\phi_8}{2} \mathbf{A} \mathbf{E} \mathbf{b} + \frac{\phi_8}{2} \mathbf{E} \mathbf{A} \mathbf{b}). \end{cases} \quad (4.36)$$

16 Since the problem is in-plane, it is convenient to introduce a parametrization  
17 in terms of the remodeling angles  $\theta_p$  and  $\theta_s$ , that is, we set  $\mathbf{a} = \cos \theta_p \mathbf{e}_1 + \sin \theta_p \mathbf{e}_2$ ,  
18  $\mathbf{b} = \cos \theta_s \mathbf{e}_1 + \sin \theta_s \mathbf{e}_2$ . In addition, without loss of generality, we can as-  
19 sume that  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$  are the principal strain directions of  $\mathbf{E}$  associated  
20 with the principal strains  $\varepsilon_1, \varepsilon_2$  and  $\varepsilon_3$ .

21 Equations (4.36) correspond therefore to the following system of scalar evo-  
22 lution equations for the angles:

$$\begin{cases} 2 m_p \dot{\theta}_p = [\phi_4 + \frac{1}{2} \phi_8 + \phi_5(\varepsilon_1 + \varepsilon_2)] (\varepsilon_1 - \varepsilon_2) \sin 2\theta_p + \frac{1}{2} \phi_8 (\varepsilon_1 + \varepsilon_2) \sin [2(\theta_p - \theta_s)], \\ 2 m_s \dot{\theta}_s = [\phi_6 + \frac{1}{2} \phi_8 + \phi_7(\varepsilon_1 + \varepsilon_2)] (\varepsilon_1 - \varepsilon_2) \sin 2\theta_s + \frac{1}{2} \phi_8 (\varepsilon_1 + \varepsilon_2) \sin [2(\theta_s - \theta_p)], \end{cases} \quad (4.37)$$

23 to be solved with the initial conditions  $\theta_p(0) = \theta_{p0}$  and  $\theta_s(0) = \theta_{s0}$ , in which  
24  $\theta_{p0}, \theta_{s0}$  are the referential primary and secondary orientation angles.

25 The following observations are duly noted:

- 1 1. depending on the representation form of the elastic strain energy, the  
2 strain component  $\varepsilon_3$  of  $\mathbf{E}$  may or may not enter the equations (4.37);  
3 indeed,  $\varepsilon_3$  does not appear explicitly, but it may be included in one of  
4 the energy derivatives  $\phi_i$ ,  $i = 4 \dots 8$ . For the sake of simplicity, in the  
5 following we will assume  $\varepsilon_3 = 0$ ;
- 6 2. the directions of principal strain  $\mathbf{e}_1$ ,  $\mathbf{e}_2$ , that correspond to  $\theta_p = k\frac{\pi}{2}$  and  
7  $\theta_s = j\frac{\pi}{2}$  ( $k, j = 0, 1, 2 \dots$ ) are stationary solutions of the remodelling  
8 equations (4.37);
- 9 3. if  $\varepsilon_1 = \varepsilon_2 = \varepsilon$ , i.e., the deformation is equibiaxial, the system of  
10 equations (4.37) simplifies into

$$\begin{cases} m_p \dot{\theta}_p = \frac{1}{2} \phi_8 \varepsilon \sin [2(\theta_p - \theta_s)] \\ m_s \dot{\theta}_s = \frac{1}{2} \phi_8 \varepsilon \sin [2(\theta_s - \theta_p)] \end{cases} \quad (4.38)$$

11 and the stationary solutions are achieved either if  $\phi_8(\varepsilon, \theta_p, \theta_s) = 0$  or if  
12  $\sin 2(\theta_p - \theta_s) = 0$ . The latter condition means that  $\Delta\theta = \theta_s - \theta_p = k\frac{\pi}{2}$   
13 ( $k = 0, 1, \dots$ ), i.e., the fibers become either parallel or orthogonal, yet  
14 their “absolute” angle with respect to  $\mathbf{e}_1$  remains undetermined. On  
15 the other hand, if  $\phi_8 = 0$  identically, meaning that the energy does not  
16 depend on  $J_8$ , then no remodeling occurs, as found also for transversely  
17 isotropic materials [36].

18 To solve the remodeling problem (4.37) and make comparisons with ex-  
19 periments, an *ansatz* on the strain energy function shall be made. In this  
20 respect, one could consider the most general form of the strain energy func-  
21 tion which is quadratic in the deformation measures. To do so, we generalize  
22 the well-known Saint Venant–Kirchhoff model, that in its original formula-  
23 tion only depends on the isotropic invariants, to a double-fibered material  
24 [50, 51]. The minimal representation of that energy which provides the sim-  
25 plest coupling between the fibers and allows to fit data from experiments on  
26 biaxial tests is:

$$\begin{aligned} \hat{\phi}(J_1, \dots, J_8) = & \frac{1}{2} k_1 J_1^2 + k_2 J_2 + \frac{1}{2} k_4 J_4^2 + \frac{1}{2} k_6 J_6^2 + \\ & + k_{14} J_1 J_4 + k_{16} J_1 J_6 + \frac{1}{2} k_8 J_8^2. \end{aligned} \quad (4.39)$$

With these assumptions, the remodelling problem takes the following form:

$$2 m_p \dot{\theta}_p = (1+r)\varepsilon_1^2 F(\theta_p, r; k_4, k_{14}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_p, \theta_s, r) + H(\theta_p, \theta_s, r)] , \quad (4.40)$$

$$2 m_s \dot{\theta}_s = (1+r)\varepsilon_1^2 F(\theta_s, r; k_6, k_{16}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_s, \theta_p, r) + H(\theta_s, \theta_p, r)] , \quad (4.41)$$

where we have introduced the biaxiality ratio  $r := -\varepsilon_2/\varepsilon_1$  between the transverse and longitudinal deformation, while the functions  $F$ ,  $G$  and  $H$  are defined as

$$F(\theta_p, r; k_4, k_{14}) := (k_4(\cos^2 \theta_p - r \sin^2 \theta_p) + k_{14}(1-r)) \sin 2\theta_p , \quad (4.42)$$

$$G(\theta_p, \theta_s, r) := 2(1-r) \cos^2(\theta_p - \theta_s) (\cos \theta_p \cos \theta_s - r \sin \theta_p \sin \theta_s) \sin(\theta_p - \theta_s) , \quad (4.43)$$

$$H(\theta_p, \theta_s, r) := (1+r) \cos(\theta_p - \theta_s) (\cos \theta_p \cos \theta_s - r \sin \theta_p \sin \theta_s) \sin 2\theta_p . \quad (4.44)$$

1 A discussion of the reorientation dynamics prescribed by the equations above  
 2 is postponed to Section 6, where inspired by experiments on cell layers we  
 3 will be able to estimate some of the constitutive coefficients ( $k_4, k_{14}, k_6, k_{16}, k_8$ ).  
 4

5 *Remark.* The representation form of the equations (4.40) and (4.41) suggests  
 6 to identify a system of elastic actions which contribute to the time rate of  
 7 the fiber orientation angles  $\theta_p$  and  $\theta_s$ . Firstly, we introduce the pair

$$\tau_p := (1+r)\varepsilon_1^2 F(\theta_p, r; k_4, k_{14}) \quad \text{and} \quad \tau_s := (1+r)\varepsilon_1^2 F(\theta_s, r; k_6, k_{16}) . \quad (4.45)$$

8 Then, we note that

$$G(\theta_s, \theta_p, r) = -G(\theta_p, \theta_s, r) . \quad (4.46)$$

9 As a consequence, we can identify the following mutual elastic interaction  
 10 between the fibers:

$$\tau_{ps} := \frac{1}{2}\varepsilon_1^2 k_8 G(\theta_p, \theta_s, r) , \quad (4.47)$$

11 dependent upon the constitutive coefficient  $k_8$ . In addition, we can define

$$\tau_{Hp} := \frac{1}{2}\varepsilon_1^2 k_8 H(\theta_p, \theta_s, r) \quad \text{and} \quad \tau_{Hs} := \frac{1}{2}\varepsilon_1^2 k_8 H(\theta_s, \theta_p, r) . \quad (4.48)$$

1 With this on hand, the remodeling equations are restated as

$$2m_p \dot{\theta}_p = \tau_p + \tau_{ps} + \tau_{Hp} \quad \text{and} \quad 2m_s \dot{\theta}_s = \tau_s - \tau_{ps} + \tau_{Hs}, \quad (4.49)$$

2 which have the following physical interpretation: the time evolution of the  
 3 orientation of the primary (resp. secondary) angle depends on the elastic  
 4 actions  $\tau_p$  (resp.  $\tau_s$ ),  $\tau_{Hp}$  (resp.  $\tau_{Hs}$ ) and  $\tau_{ps}$  (resp.  $-\tau_{ps}$ ).  $\tau_p$  is defined in  
 5 Eq. (4.45) and depends on the orientation  $\theta_p$  (resp.  $\theta_s$ ) of the fiber itself  
 6 and on the stretches  $\varepsilon_1, \varepsilon_2$ . On the other hand, the interactions  $\tau_{ps}$  and  $\tau_{Hp}$   
 7 (resp.  $\tau_{Hs}$ ) depend on both the orientations  $\theta_p$  and  $\theta_s$  and vanish when the  
 8 two fiber families are uncoupled, that is when  $k_8$  is zero.

9 It is of particular interest the evaluation of  $\tau_p, \tau_s, \tau_{Hp}, \tau_{Hs}$  and  $\tau_{ps}$  when  
 10 the stretch is equibiaxial, i.e., for  $r = -1$ , and then  $\varepsilon_1 = \varepsilon_2 = \varepsilon$ . In such a  
 11 case, Eqs. (4.43), (4.47) and (4.48) imply  $\tau_p = \tau_s = \tau_{Hp} = \tau_{Hs} = 0$  and

$$\tau_{ps} = 2k_8 \varepsilon^2 \cos^3(\theta_p - \theta_s) \sin(\theta_p - \theta_s), \quad (4.50)$$

12 meaning that the only non-zero term in the right-hand side of (4.49) is  $\tau_{ps}$ .  
 13 Since stationarity under equibiaxial stretch is attained if  $\sin 2(\theta_p - \theta_s) = 0$ ,  
 14 Eq. (4.50) states that the stationary value of the elastic interaction is zero.

## 15 5. Constrained reorientation

16 There may be practical cases in which the rotation of a fiber family  
 17 induces the same rotation in the other family, in the sense that, during  
 18 the remodeling process, the difference between the reoriented fiber angles  
 19 remains the same. This behaviour is introduced in the modeling framework  
 20 detailed above by properly constraining the elastic energy with a Lagrange  
 21 multiplier. Among the many possible choices (see for instance [52]), guided  
 22 by the experiments in [22] in which the *relative orientation* is fixed, we  
 23 require that the primary  $\mathbf{R}_p$  and secondary  $\mathbf{R}_s$  rotation tensors are equal  
 24 at any time instant. As such, we introduce the representation of rotation  
 25 tensors through the exponential maps  $\mathcal{B}_r \times \mathcal{T} \rightarrow \text{Skw}$  [52] given by

$$\mathbf{R}_p = \exp \boldsymbol{\Omega}_p \quad \text{and} \quad \mathbf{R}_s = \exp \boldsymbol{\Omega}_s. \quad (5.51)$$

26 Then,  $\boldsymbol{\Omega}_p = \boldsymbol{\Omega}_s$  implies  $\mathbf{R}_p = \mathbf{R}_s$ , and the constraint expression takes the  
 27 form

$$\mathbf{c}(\boldsymbol{\Omega}_p, \boldsymbol{\Omega}_s) = \boldsymbol{\Omega}_p - \boldsymbol{\Omega}_s, \quad (5.52)$$

28 with the corresponding constrained energy given by

$$\tilde{\varphi}(\mathbf{E}, \mathbf{A}, \mathbf{B}) = \phi(\mathbf{E}, \mathbf{A}, \mathbf{B}) + \mathbf{K} \cdot \mathbf{c}(\boldsymbol{\Omega}_p, \boldsymbol{\Omega}_s). \quad (5.53)$$

1 Hence, the skew tensor field  $\mathbf{K}$  is the Lagrange multiplier, which physically  
 2 represents the reaction needed to maintain the relative rotation between the  
 3 two fiber families the same. Equation (5.52) implies

$$\dot{\mathbf{c}}(\mathbf{R}_p, \mathbf{R}_s) = \dot{\mathbf{R}}_p \mathbf{R}_p^T - \dot{\mathbf{R}}_s \mathbf{R}_s^T. \quad (5.54)$$

On substituting (5.52) and (5.53) into the dissipation inequality, we arrive at

$$\begin{aligned} & \left( -\mathbf{S} + \mathbf{F} \frac{\partial \phi}{\partial \mathbf{E}} \right) \cdot \dot{\mathbf{F}} + \dot{\mathbf{K}} \cdot \mathbf{c}(\boldsymbol{\Omega}_p, \boldsymbol{\Omega}_s) \\ & + \left( -\boldsymbol{\Sigma}_p + \left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] + \mathbf{K} \right) \cdot \dot{\mathbf{R}}_p \mathbf{R}_p^T \\ & + \left( -\boldsymbol{\Sigma}_s + \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] - \mathbf{K} \right) \cdot \dot{\mathbf{R}}_s \mathbf{R}_s^T \leq 0, \end{aligned}$$

4 which leads to the following system of *constrained* remodelling equations:

$$\begin{cases} \mathbb{D}_p \dot{\mathbf{R}}_p \mathbf{R}_p^T = -\left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] - \mathbf{K}, \\ \mathbb{D}_s \dot{\mathbf{R}}_s \mathbf{R}_s^T = -\left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right] + \mathbf{K}, \\ \mathbf{c}(\boldsymbol{\Omega}_p, \boldsymbol{\Omega}_s) = \mathbf{0}. \end{cases} \quad (5.55)$$

5 Summing up the first two equations in (5.55), we obtain an evolution equa-  
 6 tion independent of the Lagrange multiplier  $\mathbf{K}$ :

$$\mathbb{D}_p \dot{\mathbf{R}}_p \mathbf{R}_p^T + \mathbb{D}_s \dot{\mathbf{R}}_s \mathbf{R}_s^T = -\left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right] - \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right]$$

7 which, at stationarity, gives

$$\left[ \frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A} \right]^* + \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right]^* = \mathbf{0} = [\mathbf{E}, \mathbf{S}_c]^*, \quad (5.56)$$

8 recovering the result in Eq. (3.31). On the other hand, by subtracting (5.55)<sub>1</sub>  
 9 from (5.55)<sub>2</sub> and using (5.56), at stationarity we obtain

$$\mathbf{K}^* = \left[ \frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B} \right]^*. \quad (5.57)$$

10 which furnishes the stationary values of the Lagrange multiplier  $\mathbf{K}^*$ . Equa-  
 11 tions (5.56), (5.57) together with the constraint equation (5.55)<sub>3</sub> are a sys-  
 12 tem of nine equations. The nine unknowns are the six components  $(a_i, b_i)$

1 ( $i = 1, 2, 3$ ) and the three independent components of  $\mathbf{K} \in \text{Skw}$ . Therefore,  
 2 in this constrained case, the equivalence between coaxiality of stress and  
 3 strain and stationarity of the solutions of the remodeling equation is recov-  
 4 ered thanks to the introduction of the multiplier  $\mathbf{K}$ . Indeed, if  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$   
 5 is a pair of rotations compatible with the constraint that makes stress and  
 6 strain coaxial, then (5.56) is trivially satisfied. However, the reaction term  
 7  $\mathbf{K}$  and the constraint equation guarantee that  $(\mathbf{R}_p^*, \mathbf{R}_s^*)$  is also a stationary  
 8 solution, as it is possible to find a value of  $\mathbf{K}^*$  satisfying Eq. (5.57) once  $\mathbf{a}^*$   
 9 and  $\mathbf{b}^*$  are known.

### 10 5.1. In-plane remodeling under constraint

11 When in-plane remodeling is considered, we set  $\boldsymbol{\Omega}_p = (\theta_p - \theta_{p0}) \star \mathbf{e}_3$  and  
 12  $\boldsymbol{\Omega}_s = (\theta_s - \theta_{s0}) \star \mathbf{e}_3$ , where the operator  $\star : \mathcal{V} \rightarrow \text{Skw}$  associates to each  
 13 vector  $\mathbf{w}$  a skew tensor  $\mathbf{W}$  whose axial vector is  $\mathbf{w}$ , i.e.  $(\star \mathbf{w})\mathbf{u} = \mathbf{w} \times \mathbf{u}$  for  
 14 any  $\mathbf{u} \in \mathcal{V}$ . With this notation, we have  $\mathbf{K} = \kappa \star \mathbf{e}_3$ . As a consequence, the  
 15 constraint reduces to

$$c(\theta_p, \theta_s) = (\theta_p - \theta_s) - (\theta_{p0} - \theta_{s0}), \quad (5.58)$$

whence the remodeling equations become

$$\left\{ \begin{array}{l} 2m_p \dot{\theta}_p = (1+r)\varepsilon_1^2 F(\theta_p, r; k_4, k_{14}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_p, \theta_s, r) + H(\theta_p, \theta_s, r)] - 2\kappa \\ 2m_s \dot{\theta}_s = (1+r)\varepsilon_1^2 F(\theta_s, r; k_6, k_{16}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_s, \theta_p, r) + H(\theta_s, \theta_p, r)] + 2\kappa \\ \theta_p - \theta_s = \theta_{p0} - \theta_{s0}. \end{array} \right. \quad (5.59)$$

16 The constraint equation (5.59)<sub>3</sub> implies

$$\dot{\theta}_p - \dot{\theta}_s = 0$$

from which by summing and subtracting (5.59)<sub>1</sub> and (5.59)<sub>2</sub> we get

$$\begin{aligned} 2(m_p + m_s)\dot{\theta}_p &= (1+r)\varepsilon_1^2 [F(\theta_p, r; k_4, k_{14}) + F(\theta_s, r; k_6, k_{16})] \\ &\quad + \frac{1}{2}\varepsilon_1^2 k_8 [H(\theta_p, \theta_s, r) + H(\theta_s, \theta_p, r)] \end{aligned} \quad (5.60)$$

and

$$\begin{aligned} 2(m_p - m_s)\dot{\theta}_p &= (1+r)\varepsilon_1^2 [F(\theta_p, r; k_4, k_{14}) - F(\theta_s, r; k_6, k_{16})] \\ &\quad + \frac{1}{2}\varepsilon_1^2 k_8 [2G(\theta_p, \theta_s, r) + H(\theta_p, \theta_s, r) - H(\theta_s, \theta_p, r)] - 4\kappa, \end{aligned} \quad (5.61)$$

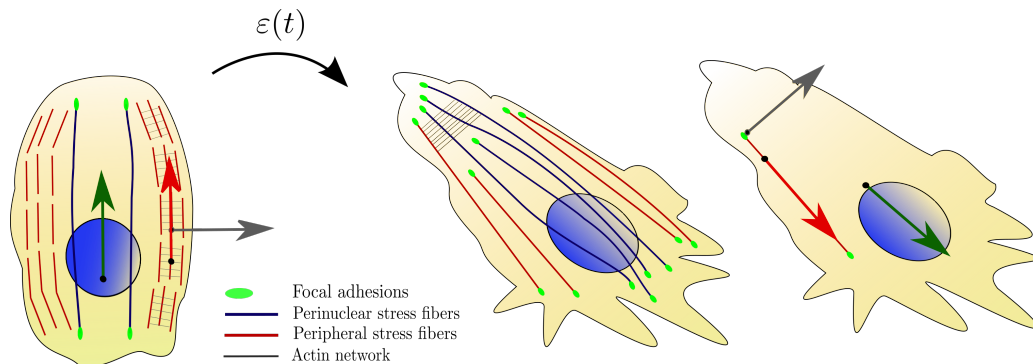


Figure 2: Sketch of the cell structure and reorientation process. For comparison with experimental assays in [22], following [30], we consider the reorientation of the actin peripheral stress fibers (in red) which determine the alignment of the cell body, while the lateral protein network (in gray) is constrained to remain orthogonal to the SF. Instead, to compare our model with results in [29], we consider the peripheral stress fibers as the primary structure, whose orientation is changed according to  $\mathbf{R}_p$ , while the nucleus and the perinuclear stress fibers (in blue) that drive its orientation represent the secondary structure, evolving with  $\mathbf{R}_s$ .

- 1 respectively, recalling (4.46). When the deformation is equibiaxial,  $r = -1$   
 2 and by using the definitions of the functions  $F$ ,  $G$  and  $H$ , Eq. (5.60) gives

$$2(m_p + m_s)\dot{\theta}_p = 0, \quad (5.62)$$

- 3 thus  $\dot{\theta}_s = \dot{\theta}_p = 0$  and no evolution occurs as happened in the transversely  
 4 isotropic case [36]. Moreover, Eq. (5.61) gives

$$\kappa = k_8 \varepsilon_1^2 \cos^3(\theta_{p0} - \theta_{s0}) \sin(\theta_{p0} - \theta_{s0}) \quad (5.63)$$

- 5 and shows that the reaction  $\kappa$  is zero either for fibre initially parallel, i.e.,  
 6  $\theta_{p0} - \theta_{s0} = k\pi$ , or orthogonal, i.e.,  $\theta_{p0} - \theta_{s0} = \frac{\pi}{2} + k\pi$  ( $k = 0, 1, \dots$ ).

- 7 *Remark.* Other choices for the constraint (5.52) are indeed possible. One  
 8 based on constraining the squared inner product between fiber vectors is  
 9 presented and discussed in the Appendix.

## 10 6. Examples from Biology

- 11 In this Section, we illustrate some applications of our framework in the  
 12 field of biology, which allow us to discuss interesting implications of the  
 13 model and to make a comparison with experimental data. In particular, we

1 focus on describing cell orientation under stretch: as mentioned in the In-  
 2 troduction, when a monolayer of cells is stretched biaxially, a reorientation  
 3 happens until each cell finds a stable configuration, characterized by a cer-  
 4 tain angle with respect to the direction of greatest stretch. For more details  
 5 on the biology and mechanics of this phenomenon, we refer the reader to  
 6 [22, 27, 28, 30, 53] and references therein.

### 7 6.1. The case of constrained reorientation

8 Livne and coworkers [22] firstly proposed a model of cell orientation  
 9 based on the minimization of the stored elastic energy with respect to the  
 10 angle between the cell and the stretching direction. Later, a generalization  
 11 of their results using a nonlinear orthotropic energy was presented in [30],  
 12 with the two fiber families representing the cell aligned stress fibers and  
 13 the orthogonal linking protein network, as sketched in Figure 2. In the  
 14 following, we show that our model is able to recover the results in [22, 30]  
 15 as a particular case, without the need of any phenomenological justification  
 16 of the evolution equation.

17 As a starting point, following [30], we consider the cell monolayer as an  
 18 hyperelastic anisotropic material, characterized by the strain energy function  
 19 defined in Eq. (4.39). Then, we introduce the two assumptions also (implic-  
 20 itly) done in [22]: (1) the families of fibers are orthogonal in the reference  
 21 configuration and constrained to remain orthogonal during remodeling; and  
 22 (2) the fibers lie in the plane of unit normal  $\mathbf{e}_3$ . Finally, we consider a  
 23 deformation of the substrate defined by  $\mathbf{E} = \text{diag}(\varepsilon_1, -r\varepsilon_1, 0)$ .

24 In doing so, we are able to apply the constrained in-plane remodeling  
 25 theory derived in Section 5.1 and to write the reorientation equations using  
 26 (5.59). Taking into account that  $\theta_{p0} - \theta_{s0} = \pi/2$ , the constraint becomes  
 27  $c(\theta_p, \theta_s) = (\theta_p - \theta_s) - \pi/2 = 0$ , which also implies  $\dot{c}(\theta_p, \theta_s) = \dot{\theta}_p - \dot{\theta}_s = 0$ .  
 28 Moreover, the orthogonality of the fibers yields

$$G(\theta_p, \theta_s, r) = G(\theta_s, \theta_p, r) = 0 \quad \text{and} \quad H(\theta_p, \theta_s, r) = H(\theta_s, \theta_p, r) = 0,$$

29 and the remodeling equations are simplified as

$$\begin{cases} 2m_p \dot{\theta}_p = (1+r)\varepsilon_1^2 F(\theta_p, r; k_4, k_{14}) - 2\kappa, \\ 2m_s \dot{\theta}_s = (1+r)\varepsilon_1^2 F(\theta_s, r; k_6, k_{16}) + 2\kappa. \end{cases} \quad (6.64)$$

30 Summing up the two equations and exploiting the constraint, we can  
 31 obtain an evolution equation for the cell orientation  $\theta_p$ :

$$\hat{m} \dot{\theta}_p = (1+r)\varepsilon_1^2 \left[ \hat{k}_p (\cos^2 \theta_p - r \sin^2 \theta_p) + k_m (1-r) \right] \sin 2\theta_p, \quad (6.65)$$



1 where

$$\widehat{m} := 2(m_p + m_s), \quad \widehat{k}_p := k_4 + k_6, \quad k_m := k_{14} - k_{16} - k_6.$$

2 The stationary solutions of Eq. (6.65) can be readily identified: they corre-  
 3 spond either to the cell being aligned with the principal directions of strain,  
 4 i.e.  $\theta_p^* = k\pi/2, k \in \mathbb{Z}$ , or to the oblique orientations defined by

$$\cos^2 \theta_p^* = 1 + \frac{k_m}{\widehat{k}_p} - \frac{1}{1+r} \left( 1 + 2 \frac{k_m}{\widehat{k}_p} \right) = \frac{1}{2} + \mathcal{K} \left( \frac{1}{2} - \frac{1}{1+r} \right), \quad (6.66)$$

5 where  $\mathcal{K} := 1 + 2k_m/\widehat{k}_p$ . Such a result is coherent with previous findings  
 6 characterizing the preferential orientations of cells on a stretched substrate,  
 7 both in linear elasticity [22], nonlinear elasticity [30] and viscoelasticity [31].  
 8 However, in our model we did not postulate the evolution equation (6.65)  
 9 as done in previous works, but rather derived it from a more general frame-  
 10 work lying on balance principles and thermodynamics. Clearly, the oblique  
 11 stationary solutions only exist when  $r \neq -1$  and the right-hand side of  
 12 Eq. (6.66) has a value between 0 and 1; for details on the bifurcation anal-  
 13 ysis of the orientations, see [30].

14 The Lagrange multiplier  $\kappa$ , that represents the reaction needed to keep  
 15 the fibers orthogonal, can be evaluated at stationarity through

$$4\kappa^* = (1+r)\varepsilon_1^2 [(k_4 - k_6)(\cos^2 \theta_p^* - r \sin^2 \theta_p^*) + (k_{14} + k_{16} + k_6)(1 - r)] \sin 2\theta_p^*. \quad (6.67)$$

16 We observe that, when the cell is aligned with the principal strain directions,  
 17  $\kappa^* = 0$ . Indeed the same holds true when  $r = -1$  (see (6.65)), i.e. in the  
 18 case of equibiaxial deformation when no reorientation occurs. For oblique  
 19 orientations, instead, we have

$$4\kappa^* = 2(1 - r^2)\varepsilon_1^2 \frac{k_4 k_{16} + k_4 k_6 + k_6 k_{14}}{k_4 + k_6} \sin 2\theta_p^*, \quad (6.68)$$

20 which is in general different from zero provided that  $r \neq 1$ .

21 We conclude this Section by comparing the prediction of the constrained  
 22 model with the data on cell reorientation in [22]. It is seen from Eq. (6.65),  
 23 that the three parameters  $\widehat{k}_p, k_m$  and  $\tau$ , where the latter is the characteris-  
 24 tic time in  $\widehat{m}$ , have to be calibrated. The results of this procedure, carried  
 25 out through a nonlinear least square algorithm, are shown in Figure 3. The  
 26 model matches accurately the evolution of the orientation angles seen in the  
 27 experiments with a relative error below 2 %. The optimal parameters used

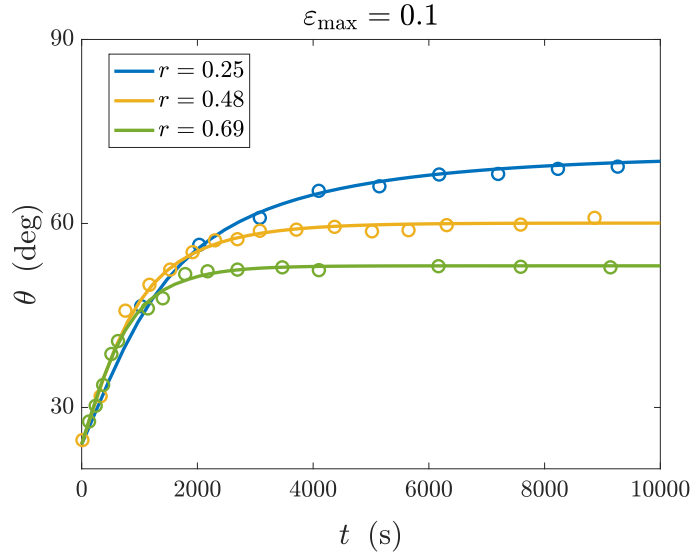


Figure 3: Evolution of the cell orientation angle  $\theta_p$  with maximum strain of 10%, following Eq. (6.65), for different values of the biaxiality ratio  $r$ . The curves show the best fitting of the model, while the dots represent experimental data taken from [22].

$r$	$k_m/\widehat{k}_p$	$\tau$ [s]
0.25	0.1594	7.3
0.48	0.2142	5.9
0.69	0.2596	5.7

Table 1: Constitutive parameters in Eq. (6.65) estimated from the fitting of experiments in [22].

1 for the fitting for  $r \in \{0.25, 0.48, 0.69\}$  are listed in Table 1 and are indeed  
 2 coherent with experiments in [22], where the authors found a value of the  
 3 ratio  $k_m/\widehat{k}_p = 0.13 \pm 0.04$  and a characteristic time  $\tau = 6.6 \pm 0.4$  s.  
 4 It is worth noting that the evolution of the angle in Eq. (6.65) only depends  
 5 on three constitutive parameters including a characteristic time. The eval-  
 6 uation of the other model coefficients, necessary to estimate the Lagrange  
 7 multiplier  $\kappa^*$ , would require further experimental data.

8 *Remark.* In the general case of two plane fiber families constrained to remain  
 9 orthogonal, namely such that  $\mathbf{A} + \mathbf{B} = \check{\mathbf{I}}$  with  $\check{\mathbf{I}}$  the identity tensor in the  
 10 fiber plane, it can be easily shown that the stationarity requirement

$$\left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^* + \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right]^* = \mathbf{0} \quad (6.69)$$

11 implies

$$[\mathbf{E}, (\phi_4^* - \phi_6^*)\mathbf{A}^* + (\phi_5^* - \phi_7^*)(\mathbf{A}^*\mathbf{E} + \mathbf{E}\mathbf{A}^*)] = \mathbf{0}, \quad (6.70)$$

12 which has the following consequences:

- 13 1. If  $\phi_6 = \phi_7 = 0$  identically, meaning that there is a single fiber family,  
 14 the relation  $[\mathbf{E}, \mathbf{S}_c^*] = \mathbf{0}$  for a transversely isotropic material found in  
 15 [36] is recovered.
- 16 2. If the remodeled direction  $\mathbf{a}$  is along a principal direction of strain  
 17 (and then so is  $\mathbf{b}$  because they are orthogonal), the commutator on the  
 18 l.h.s. of (6.70) is null. Therefore, rotations that align the preferential  
 19 orientations with the principal strain directions are always stationary  
 20 solutions of the problem at hand.
- 21 3. If  $\mathbf{a}$  is not aligned with a principal strain direction, there might be  
 22 additional non-trivial solutions identified by the two conditions

$$\phi_4^*(\mathbf{E}, \mathbf{A}^*) = \phi_6^*(\mathbf{E}, \mathbf{A}^*) \quad \text{and} \quad \phi_5^*(\mathbf{E}, \mathbf{A}^*) = \phi_7^*(\mathbf{E}, \mathbf{A}^*).$$

### 23 6.2. The case of independent reorientation

24 The complex interaction between the cell nucleus and the cytoplasm can  
 25 be still captured by the proposed model in terms of changes in their relative  
 26 orientation when cells are cyclically stretched.

27 In [29], the mechanoadaptive organization of stress fibers and nuclei in ep-  
 28 ithelial cells under cyclic stretches is considered, highlighting that these two  
 29 cellular components follow different orientation dynamics. In particular, ep-  
 30 ithelial cells on a plane substrate were stretched for 2 hours at 5%, 10% and

Table 2: Constitutive parameters in Eqs. (4.40)-(4.41) identified from the experiments in [29].

$k_{14}/k_4$	$k_{16}/k_6$	$k_6/k_4$	$k_8/k_4$	$\tau_p$ [s]	$\tau_s$ [s]
26.5	3.3	9.75	75	128	185

1 15% maximum strains whilst measuring the reorientation of the different  
 2 stress fiber subtypes. It was seen that dorsal stress fibers, transverse arcs,  
 3 and peripheral stress fibers were mainly involved in the cytoplasm response  
 4 whereas perinuclear cap fibers were associated with the reorientation and  
 5 elongation of the nucleus (see Fig. 2).

6 A sketch of the experimental setup of [29] is shown in Fig. 4(a) where  
 7 the coloured arrows are used to indicate the primary (red) and secondary  
 8 (green) cell structures, i.e., cytoplasm and nucleus of the cell, respectively.  
 9 In the experiments, the longitudinal strain  $\varepsilon_1$  was controlled for 2 hours  
 10 with the time history shown in inset 4(b) at two different level of maximum  
 11 strain (10% and 15%); the lateral strain was also controlled in a way that  
 12  $r = -\varepsilon_2/\varepsilon_1 = 0.49$  and the frequency of the deformation was set to 0.3 Hz.  
 13 The corresponding reorientation velocities are shown in Fig. 4(c) for the  
 14 primary  $\dot{\theta}_p$  and the secondary angle  $\dot{\theta}_s$ . These graphs were obtained by  
 15 fitting the experimental data against Eqs. (4.40)-(4.41) (with  $m_p = k_4\tau_p$   
 16 and  $m_s = k_6\tau_s$ ), through a nonlinear least square algorithm implemented in  
 17 MATLAB<sup>®</sup>. The corresponding best fit parameters are listed in Table 2.

18 It is pointed out that the experimental results at 5% were not used for  
 19 the fitting process, since they did not show any significant reorientation,  
 20 probably caused by the poor interaction between cells and substrate at such  
 21 a low level of strain. Finally, Figs. 4(d)-(e) show the evolution of the average  
 22 orientation angles during the 2 hours test. [The stretch dependence for both  
 23 the primary and secondary angles is well captured by the model with a  
 24 maximum relative error of 2.5% only seen for the nucleus in inset \(e\).](#) The  
 25 fitting is achieved with a value of the constitutive parameter  $k_8$  significantly  
 26 larger than  $k_4$  and  $k_6$ , indicating a strong interaction between the two fibre  
 27 families.

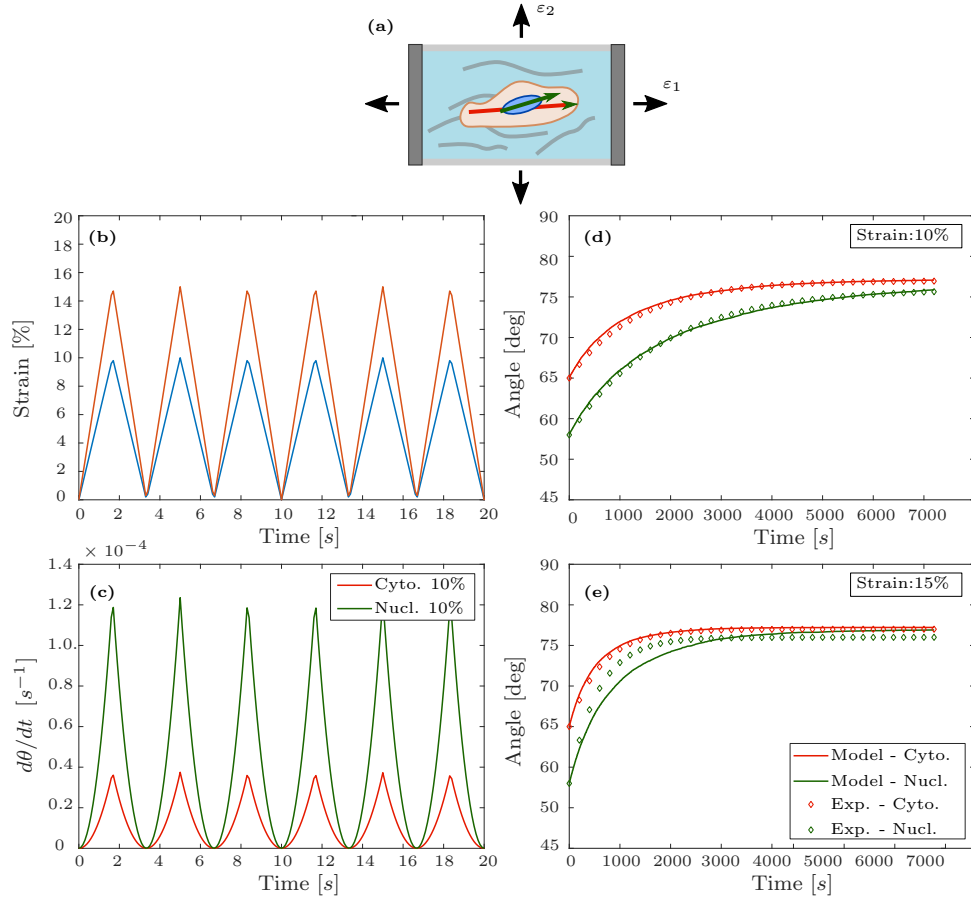


Figure 4: (a): Sketch of the experiments in [29], where the substrate is deformed with a periodic strain. (b): Time history of the longitudinal strain  $\varepsilon_1$  imposed to the substrate, with maximum amplitude of 10% (blue curve) and 15% (orange curve). (c): Angular velocity of reorientation for the primary and secondary structures obtained from the model with the optimal estimated constitutive parameters in Tab. 2. (d)–(e): Evolution of the average (over a cycle) orientation angle during the test for the maximum strain 10% (d) and 15% (e), for both the cytoplasm and the nucleus, compared with experimental results in [29].

## 1 7. Conclusions

2 We presented a model to describe cell alignment under applied trac-  
3 tion using a fiber reorientation framework, in which two different families  
4 of fibers are able to rotate independently under the action of two distinct  
5 rotation tensors. The framework accounts for the elastic coupling between  
6 the fiber families, while the introduction of a proper constraint allowed us  
7 to recover some literature results on reorientation of transversely isotropic  
8 and orthotropic materials. The stationary solutions of the remodelling equa-  
9 tions are then thoroughly studied to find a generalization of a well-known  
10 coaxiality theorem by Vianello, that holds in the passive case; active effects,  
11 even if not studied in details in the present paper, can be naturally and  
12 straightforwardly incorporated in the modelling equations.

13 As a main application of the proposed framework, we studied cell reorienta-  
14 tion under stretch. Perfect adhesion is assumed between the cell layer and  
15 the substrate and the rotations of the cells due to mechanical stimuli are  
16 viewed as additional state variables of the problem. By using experimental  
17 data available from the literature, we have found that the model is able to  
18 accurately match the experimental results on cell orientation for both the  
19 constrained and unconstrained fiber evolutions. Even though the focus is  
20 mainly on biological applications, the proposed framework is indeed general.  
21 As such, it could be readily adapted to describe engineering materials like  
22 composites with two families of fibers [54], which are engineered to reorient  
23 under different stimuli.

24 The thermodynamically consistent structure of the model offers advantages  
25 over the existing phenomenological approaches pursued in the literature and  
26 may open the road to future developments. These include: the possibility  
27 of having a mobility tensor dependent both on time and on strain so to  
28 describe the dynamic response seen for certain types of cells [55, 56]; the  
29 incorporation of a non-perfect adhesion between cells and substrate by in-  
30 ducing reorientation only when a certain amount of strain is accumulated  
31 [55] or when adhesion bonds are broken as a consequence of mechanical de-  
32 formation; the inclusion of the matrix viscoelasticity, that in general induces  
33 additional characteristic times in the material response. The hierarchic role  
34 of the fiber families may also be incorporated by distinguishing between  
35 “pulled” and “dragged” reorientations, that occur when one fiber family  
36 drives the reorientation of the other through the elastic coupling.

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## 22 **Appendix A. An alternative choice for the constraint equation**

23 Here we consider the alternative choice of the scalar constraint

$$c(\mathbf{A}, \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} - \mathbf{A}_0 \cdot \mathbf{B}_0, \quad (\text{A.1})$$

24 which gives

$$\dot{c}(\mathbf{A}, \mathbf{B}) = \dot{\mathbf{A}} \cdot \mathbf{B} + \mathbf{A} \cdot \dot{\mathbf{B}} = [\mathbf{A}, \mathbf{B}] \cdot (\dot{\mathbf{R}}_s \mathbf{R}_s^T - \dot{\mathbf{R}}_p \mathbf{R}_p^T). \quad (\text{A.2})$$

25 Accordingly, following the procedure detailed in Section 5, the evolution  
26 equations of the constrained remodeling problem are written as

$$\left\{ \begin{array}{l} \mathbb{D}_p \dot{\mathbf{R}}_p \mathbf{R}_p^T = -\left[\frac{\partial \phi}{\partial \mathbf{A}}, \mathbf{A}\right] + \kappa [\mathbf{A}, \mathbf{B}], \\ \mathbb{D}_s \dot{\mathbf{R}}_s \mathbf{R}_s^T = -\left[\frac{\partial \phi}{\partial \mathbf{B}}, \mathbf{B}\right] - \kappa [\mathbf{A}, \mathbf{B}], \\ \mathbf{A} \cdot \mathbf{B} = \mathbf{A}_0 \cdot \mathbf{B}_0, \end{array} \right. \quad (\text{A.3})$$

- 1 having introduced a scalar Lagrange multiplier  $\kappa$ . At stationarity, summing  
 2 the two equations one gets

$$\left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^* + \left[\frac{\partial\phi}{\partial\mathbf{B}}, \mathbf{B}\right]^* = \mathbf{0} = [\mathbf{E}, \mathbf{S}_c]^* \quad (\text{A.4})$$

- 3 and subtracting instead yields

$$\kappa^* [\mathbf{A}, \mathbf{B}]^* = \left[\frac{\partial\phi}{\partial\mathbf{A}}, \mathbf{A}\right]^*. \quad (\text{A.5})$$

- 4 On assuming that  $\mathbf{a} = \cos\theta_p\mathbf{e}_1 + \sin\theta_p\mathbf{e}_2$  and  $\mathbf{b} = \cos\theta_s\mathbf{e}_1 + \sin\theta_s\mathbf{e}_2$ , the  
 5 constraint equation (A.1) gives

$$c(\mathbf{a}, \mathbf{b}) = \cos^2(\theta_p - \theta_s) - \cos^2(\theta_{p0} - \theta_{s0}), \quad (\text{A.6})$$

whence the remodeling equations become

$$\begin{cases} 2m_p\dot{\theta}_p = (1+r)\varepsilon_1^2 F(\theta_p, r; k_4, k_{14}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_p, \theta_s, r) + H(\theta_p, \theta_s, r)] + \kappa \sin(2(\theta_s - \theta_p)) \\ 2m_s\dot{\theta}_s = (1+r)\varepsilon_1^2 F(\theta_s, r; k_6, k_{16}) + \frac{1}{2}\varepsilon_1^2 k_8 [G(\theta_s, \theta_p, r) + H(\theta_p, \theta_s, r)] - \kappa \sin(2(\theta_s - \theta_p)) \\ \cos^2(\theta_p - \theta_s) = \cos^2(\theta_{p0} - \theta_{s0}). \end{cases} \quad (\text{A.7})$$

For an equibiaxial test, with  $r = -1$ , by summing and subtracting the first two equations in (A.7) one obtains

$$\begin{cases} m_p\dot{\theta}_p + m_s\dot{\theta}_s = 0 \\ m_p\dot{\theta}_p - m_s\dot{\theta}_s = \varepsilon_1^2 k_8 \cos^2(\theta_p - \theta_s) \sin(2(\theta_p - \theta_s)) - \kappa \sin(\theta_p - \theta_s) \\ \cos^2(\theta_p - \theta_s) = \cos^2(\theta_{p0} - \theta_{s0}). \end{cases} \quad (\text{A.8})$$

- 6 The constraint equation  $\cos^2(\theta_p - \theta_s) = \pm \cos^2(\theta_{p0} - \theta_{s0})$  implies that

$$\dot{c} = \sin(2(\theta_s - \theta_p))(\dot{\theta}_p - \dot{\theta}_s) = 0, \quad (\text{A.9})$$

- 7 which has the solutions  $\dot{\theta}_p = \dot{\theta}_s$  or  $\sin(2(\theta_s - \theta_p)) = 0$ , that is  $\Delta\theta = \theta_s -$   
 8  $\theta_p = (1+k)\frac{\pi}{2}$ ,  $\kappa = 0, 1, 2, \dots$ . The former substituted into (A.8) gives  
 9  $\dot{\theta}_p = \dot{\theta}_s = 0$  and  $\kappa = \varepsilon_1^2 k_8 \cos^2(\Delta\theta_0)$ . The latter gives  $\dot{\theta}_p = \dot{\theta}_s = 0$  and an  
 10 indeterminate reaction couple  $\kappa$ . In both cases, however, it is obtained that  
 11 no remodeling occurs when equibiaxial strains are considered, as already  
 12 seen from Eq. (5.59).