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An Allen–Cahn approach to the remodelling of fibre-reinforced anisotropic materials / Grillo, Alfio; Carfanga, Melania; Federico, Salvatore. - In: JOURNAL OF ENGINEERING MATHEMATICS. - ISSN 0022-0833. - STAMPA. - 109:1(2018), pp. 139-172. [10.1007/s10665-017-9940-8]

Availability: This version is available at: 11583/2683512 since: 2020-06-02T19:45:07Z

Publisher: Springer

Published DOI:10.1007/s10665-017-9940-8

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(Article begins on next page)

An Allen-Cahn Approach to the Remodelling of Fibre-Reinforced Anisotropic Materials

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6 Received: date / Accepted: date

Abstract We propose a theory of remodelling in fibre-reinforced biological 7 tissues, in which the fibre orientation follows a given probability density. The latter is characterised by variance and mean angle. We claim that the fibres may change their orientation in time, thereby triggering a remodelling process 10 that can be described by the spatiotemporal evolution of the mean angle. 11 This is determined by solving a balance of external and internal generalised 12 forces. We assign the latter ones by establishing a constitutive theory capable 13 of resolving the spatial variability of the fibre mean angle, and featuring a 14 free energy density of the Allen-Cahn type. Through numerical simulations, 15 we compare the predictions of our model with the results of another model 16 available in the literature. Finally, we interpret the evolution of the mean angle 17 as the consequence of a symmetry breaking that occurs in the tissue both 18 spontaneously and due to the coupling between remodelling and deformation. 19

Keywords Porous Media · Biological tissue · Biphasic material · Fibre reinforcement · Transverse isotropy · Remodelling · Structural changes

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This work has been supported in part by the *Politecnico di Torino* (Italy) [AG and MC], in part by the *Fondazione Cassa di Risparmio di Torino* (Italy), through the *La Ricerca dei Talenti* ("HR Excellence in Research") programme [AG and MC] and in part by the Natural Sciences and Engineering Research Council of Canada, through the NSERC Discovery Programme [SF].

22 1 Introduction

Following Cowin's terminology [1], a biological tissue is "a collection of cells"
embedded in an extracellular matrix (ECM). Among the constituents of the
ECM, elastin and collagen fibres play an essential role in determining the
mechanical properties of tissues.

In order to understand how a tissue is generated, how it works, and how it 27 adapts itself to external stimuli, it is necessary to know the internal structure of 28 the tissue itself and the mechanical behaviour of its constituents. Of particular 29 relevance is the study of the ECM, whose properties are tightly related to the 30 presence of elastin and collagen fibres, and to their spatial orientation. In the 31 case of blood vessels, several mathematical models of the tissue's mechanics 32 have been elaborated, in which a discrete number of families of fibres is con-33 sidered (see, e.g., [2–6]). Moreover, models that consider statistically oriented 34 fibres have been proposed for various tissues, for example, in [7–10]. To account 35 for the fibres in the constitutive description of biological tissues, the structure 36 tensor is included in the determination of stress through the introduction of 37 suitable invariants of the Cauchy deformation tensor [2, 11, 12]. 38

When the ECM is permeated by an interstitial fluid, the pattern of fibre 39 orientation influences the motion of the fluid by either facilitating or hindering 40 its flow. For instance, this is the case of articular cartilage, whose permeability 41 in the superficial zone should be higher than it actually is, based solely on con-42 siderations on the proteoglycan volumetric fraction, as observed by Maroudas 43 and Bullough [13]. Maroudas and Bullough [13] also inferred that this be-44 haviour was likely due to the collagen fibres, which, in the superficial zone, are 45 oriented parallel to the surface and therefore constitute a further obstacle to 46 fluid flow. A possible explanation of this occurrence has been presented in [9]. 47 Subsequently, by putting together the non-linear elasticity model presented in 48 [14], and extending to large deformations the permeability model developed in 49 [15], a general, finite-deformation model was introduced in [16]. In this series 50 of papers, the fibres are assumed to be oriented statistically according to a 51 probability density capable of mimicking the histological pattern observed by 52 other authors [17, 18]. 53

When a tissue deforms, its mechanical properties evolve in time. The de-54 55 formation, indeed, drives the reorientation of the fibres, thereby modulating the mechanical behaviour of the tissue also in response to the changes in its 56 internal structure. If the deformation is the only responsible for this structural 57 reorganisation, the evolution of the fibre pattern may be said to be a *passive* 58 consequence of the deformation. If, however, as suggested in [19], a tissue is 59 supposed to possess also structural degrees of freedom, which exist indepen-60 dently of deformation, then the reorientation of the fibres becomes part of the 61 tissue dynamics, and it *interacts* with the deformation and stress. This interac-62 tion, in turn, may manifest itself in several ways, among which a relevant one 63 is given by the identification of a *stress-driven* pattern of fibre arrangement. 64 Motivated by the aforementioned considerations, the scope of this work 65 is to propose a model of structural adaptation in fibre-reinforced biological 66

tissues. In the present framework, the "structural adaptation" is assumed to 67 consist of a variation of the material properties that determine the local ori-68 entation of the fibres in a fibre-reinforced soft tissue [20,21]. More specifically, 69 we consider a simplified theoretical setting, in which the only interactions ex-70 perienced by the tissue arise due to mechanical stimuli, and the tissue itself is 71 72 hyperelastic. Moreover, no inelastic distortions are considered. Hence, the reorientation of fibres is assumed not to be accompanied by growth, resorption, 73 or any other process of this kind. Still, dissipative entities yielding the vari-74 ation of the tissue's internal structure are taken into account. Following the 75 line of thought put forward in [22,23], a probability distribution of the fibre 76 orientation is prescribed, whose functional law features a family of parameters 77 depending on the material points and on time. These parameters shall be re-78 ferred to as *remodelling variables* in the sequel. While the dependence of the 79 remodelling variables on the material points is related to the inhomogeneity 80 of the tissue, their dependence on time is introduced here in order to allow for 81 their evolution, which is understood as a manifestation of the tissue's struc-82 tural adaptation. On this footing, we present a theory of remodelling that, 83 starting from the setup outlined in [22,23], relies on the introduction of a free 84 energy density of the Ginzburg-Landau [24,25] or Allen-Cahn [26] type, and 85 accounts explicitly for the spatial resolution of the remodelling variable¹. 86

As done in [27,22,23], the hypothesis is made that the remodelling variables are indeed "kinematic variables", for which suitable balance laws should be introduced in conjunction with the balance laws typically adopted in the continuum mechanics of simple bodies. In this respect, this vision of structural adaptation takes large inspiration from the models of Cermelli et al. [28] and DiCarlo and Quiligotti [19], in which the concept of a "two-layer dynamics" is thoroughly explained.

Previous studies on remodelling have been conducted by many other au-94 thors. For example, the interplay between the fibre alignment in fibre-reinforced 95 media and other aspects of the tissue mechanics has been highlighted in [29], 96 while remodelling in collagen gels and tissues with collagenous reinforcement 97 has been studied in [30]. In a slightly different context, a possible coupling 98 between fibre reorientation and growth has been proposed in [31], in conjunc-99 tion with the Bilby-Kröner-Lee decomposition. Furthermore, the remodelling 100 of the collagen fibres has been addressed also in [32], and the compaction of 101 collagen gels has been studied in [33]. Recently, the influence of the collagen 102 fibres on the mechanics of the aorta has been studied in [34–36]. 103

The remainder of this work is organised as follows. In Section 2, we introduce the dynamics of remodelling. In Section 3, we establish the constitutive framework. In Section 4, we study in detail the remodelling equation, and discuss its asymptotic behaviour. In Section 5, we comment the results of the numerical simulations. Finally, in Section 6, we summarise the key-points of our work, and propose an outline for future research.

¹ The idea was suggested by Prof. Gaetano Giaquinta to S. Federico, S.-K. Han, and A. Grillo during the visit of S.-K. Han to the University of Catania, in 2004, while discussing about the histology of articular cartilage.

110 2 General mathematical model

We consider a fibre-reinforced porous medium, in which the reinforcing fibres 111 are oriented statistically according to some suitable probability density. To 112 formalise the mathematical description of media of this type, we refer to the 113 works [37, 16, 38-40], which we briefly summarise here. Within the present 114 theoretical framework, the tissue is regarded as a biphasic medium comprising 115 a fluid and a solid phase. The solid phase is the representation of a porous 116 medium, which is assumed to consist of a matrix of biological polymers (e.g., 117 proteoglycans in the case of articular cartilage) and a network of collagen 118 fibres. 119

¹²⁰ 2.1 Theoretical background

At the scale at which our theory is formulated, the matrix and the collagen fibres constitute a mixture, in which they are present with volumetric fractions ϕ_{0s} and ϕ_{1s} , respectively. The sum $\phi_s = \phi_{0s} + \phi_{1s}$ defines the volumetric fraction of the solid phase as a whole and, since the saturation condition is assumed to apply, the volumetric fraction of the fluid phase coincides with the porosity of the medium and is given by $\phi_f = 1 - \phi_s$.

The portion of the three-dimensional Euclidean space, S, occupied by the 127 tissue at time t is said to be the *current configuration* of the tissue. We also 128 introduce a reference configuration, \mathcal{B} . For $x \in \mathcal{S}$ and $X \in \mathcal{B}$, we consider 129 the tangent spaces T_x S and T_X B, and the co-tangent spaces T_x^* S and T_X^* B. 130 Moreover, we denote by $TS = \bigsqcup_{x \in S} T_x S$ and $TB = \bigsqcup_{X \in B} T_X B$ the tangent 131 bundles of S and B, and by $T^*S = \bigsqcup_{x \in S} T^*_x S$ and $T^*B = \bigsqcup_{X \in B} T^*_X B$ their 132 co-tangent bundles, respectively [41]. Finally, the space S and the reference 133 configuration \mathcal{B} are endowed with the metric tensors g and G, respectively. 134

In the present framework, matrix and fibres are assumed to share the same motion. This hypothesis allows to describe the motion of the solid phase by means of a one-parameter family of smooth embeddings. At each time t, the embedding $\chi(\cdot, t)$ maps the points of \mathcal{B} into \mathcal{S} (see [37,38] for details), i.e.,

$$\chi(\cdot, t) : \mathcal{B} \to \mathcal{S}, \quad X \in \mathcal{B} \ \mapsto x = \chi(X, t) \in \mathcal{S}.$$
 (1)

The tangent map $T\chi(X,t) = \mathbf{F}(X,t) : T_X \mathcal{B} \to T_{\chi(X,t)} \mathcal{S}$ is the deformation gradient tensor of the solid phase [41], while $\mathbf{C} = \mathbf{F}^{\mathrm{T}} \mathbf{g} \mathbf{F}$ and $\mathbf{b} = \mathbf{F} \mathbf{G}^{-1} \mathbf{F}^{\mathrm{T}}$ denote the right and the left Cauchy-Green deformation tensor, respectively. In order for $\chi(X,t)$ to be admissible, $\mathbf{F}(X,t)$ is required to have strictly positive determinant, $J(X,t) = \det \mathbf{F}(X,t)$, at all points and at all times.

To complete the kinematic description of the considered porous medium, we introduce the velocities of the solid and fluid phase, $\boldsymbol{v}_{\rm s}$ and $\boldsymbol{v}_{\rm f}$, the *filtration velocity* $\boldsymbol{q} = \phi_{\rm f} \boldsymbol{w}$, with $\boldsymbol{w} = \boldsymbol{v}_{\rm f} - \boldsymbol{v}_{\rm s}$ being the relative velocity of the fluid with respect to the solid motion, and the backward Piola transformation of \boldsymbol{q} , $\boldsymbol{\Omega} = J \boldsymbol{F}^{-1} \boldsymbol{q}$, which is referred to as the *material* filtration velocity.

¹⁴⁹ 2.2 Directional averages

At the scale of a single fibre, the fibre appears as a curved cylinder whose 150 length is much larger than the diameter of the cross section. This allows to 151 model the fibre as a curve. Furthermore, in a sufficiently small neighbourhood 152 of a given point $X \in \mathcal{B}$, a fibre can be approximated by its tangent line [15], 153 which defines the local direction of fibre alignment. Such direction can be 154 associated with a unit vector, M_X , emanating from X. Since the orientation 155 of the fibres is assumed to be statistical at each point, we need to define 156 the probability density that a fibre passing by X is oriented along a given 157 direction. To this end, we introduce the set of all unit vectors of $T_X \mathcal{B}$, i.e., 158 $\mathbb{S}_X^2 \mathcal{B} = \{ M_X \in T_X \mathcal{B} : \| M_X \| = 1 \}, \text{ and the function } \Psi_X : \mathbb{S}_X^2 \mathcal{B} \to \mathbb{R}_0^+$ such that, for a given $M_X \in \mathbb{S}_X^2 \mathcal{B}, \Psi_X(M_X)$ is the probability density that 159 160 a (rectified) fibre passing from X is locally aligned along M_X . Since Ψ_X is 161 assumed to be a continuous probability density, it has to be normalised. 162

Given a physical property (e.g., a scalar one) depending on the direction of the fibres at X, and expressed thus as $\mathfrak{F}_X : \mathbb{S}^2_X \mathcal{B} \to \mathbb{R}$, the *directional average* of \mathfrak{F}_X is defined by (see, e.g., [16] and references therein)

$$\langle\!\langle \mathfrak{F}_X \rangle\!\rangle = \int_{\mathbb{S}_X^2 \mathcal{B}} \mathfrak{F}_X(\boldsymbol{M}_X) \, \Psi_X(\boldsymbol{M}_X) = \int_0^{2\pi} \int_0^{\pi} \mathfrak{F}_X(\hat{\boldsymbol{M}}_X(\Theta, \Phi)) \, \Psi_X(\hat{\boldsymbol{M}}_X(\Theta, \Phi)) \sin(\Theta) \mathrm{d}\Theta \mathrm{d}\Phi,$$
(2)

where, for $(\Theta, \Phi) \in [0, \pi] \times [0, 2\pi[$,

$$M_X = \hat{M}_X(\Theta, \Phi) = \sin \Theta \cos \Phi \, \mathcal{E}_1 + \sin \Theta \sin \Phi \, \mathcal{E}_2 + \cos \Theta \, \mathcal{E}_3, \qquad (3)$$

and $\{\mathcal{E}_I\}_{I=1}^3$ is an orthonormal vector basis of $T_X\mathcal{B}$. The second equality in (2) stems from rephrasing the integral over $\mathbb{S}_X^2\mathcal{B}$ as a surface integral and expressing it in spherical coordinates, granted that each $M_X \in \mathbb{S}_X^2\mathcal{B}$ corresponds univocally to a point on the surface of the unit sphere centred at X.

In this work, we assume that the matrix of the solid phase is isotropic and 171 that a fibre aligned along M_X at $X \in \mathcal{B}$ is transversely isotropic with respect 172 M_X . Thus, \mathfrak{F}_X must satisfy the symmetry condition $\mathfrak{F}_X(HM_X) = \mathfrak{F}_X(M_X)$, 173 for all proper rotation tensors H such that $HM_X = \pm M_X$. If there exists a 174 direction of symmetry for the whole tissue, i.e., if there exists M_0 such that 175 for all $X \in \mathcal{B}$, for all $M_X \in \mathbb{S}^2_X \mathcal{B}$, and for every proper rotation tensor H_0 176 with the property $H_0M_0 = \pm M_0$, the invariance condition $\Psi_X(H_0M_X) =$ 177 $\Psi_X(M_X)$ holds true, then the probability density is transversely isotropic 178 with respect to M_0 . Consequently, the directional average $\langle \mathfrak{F}_X \rangle$ turns out to 179 be transversely isotropic with respect to M_0 , while $\mathfrak{F}_X(M_X)$ is transversely 180 isotropic with respect to M_X . Further restrictions descend from the hypothesis 181 that the physical quantities depending on the orientation of the fibres are 182 invariant under the transformation $M_X \mapsto -M_X$, for all M_X and for all 183 $X \in \mathcal{B}$. To fulfil this property, the generic physical quantity \mathfrak{F}_X has to depend 184

on M_X through $A_X = M_X \otimes M_X$, which is referred to as *structure tensor*,

and fulfils the identity $\boldsymbol{H}\boldsymbol{A}_{X}\boldsymbol{H}^{\mathrm{T}} = \boldsymbol{A}_{X}$. Accordingly, the probability density must comply with the invariance condition $\Psi_{X}(\boldsymbol{M}_{X}) = \Psi_{X}(-\boldsymbol{M}_{X})$.

When $M_X \in \mathbb{S}^2_X \mathcal{B}$ is expressed as in (3), the transverse isotropy of Ψ_X 188 implies that $\Psi_X(\hat{M}_X(\Theta, \Phi))$ is independent of Φ , whence the possibility of in-189 troducing a function $\wp_X : [0, \pi] \to \mathbb{R}_0^+$ such that $\wp_X(\Theta) = \Psi_X(\hat{M}_X(\Theta, \Phi))$, for 190 all $\Phi \in [0, 2\pi[$. To be compatible with the restriction $\Psi_X(M_X) = \Psi_X(-M_X)$, 191 \wp_X must respect the constraint $\wp_X(\Theta) = \wp_X(\pi - \Theta)$, for all $\Theta \in [0, \pi]$. This 192 property is also satisfied by all the physical quantities studied in this work, 193 and allows thus to determine the directional averages in (2) by computing the 194 integrals over the hemisphere $\mathbb{S}_X^{2+}\mathcal{B} = \{M_X \in \mathbb{S}_X^2\mathcal{B} | M_X \cdot M_0 \ge 0\}$, i.e., 195

where $\bar{\wp}_X : [0, \pi/2] \to \mathbb{R}_0^+$ is a re-definition of \wp_X . Very often, the von Mises probability density is used when spherical data are concerned [8,10,38]. Here,

¹⁹⁸ however, for our purposes, we employ the pseudo-Gaussian density

$$\bar{\wp}_X(\Theta) = \frac{\gamma_X(\Theta)}{2\pi \int_0^{\pi/2} \gamma_X(\Theta') \sin(\Theta') d\Theta'},$$
(5a)

$$\gamma_X(\Theta) = \exp\left(-\frac{\left[\Theta - Q(X)\right]^2}{2\left[\omega(X)\right]^2}\right),\tag{5b}$$

where Q(X) and $[\omega(X)]^2$ represent the mean angle and variance of the probability density, respectively. The choice of the pseudo-Gaussian distribution is corroborated by the fact that it modelled satisfactorily the orientation of the collagen fibres in articular cartilage [9], as determined in the X-ray diffraction experiments carried out in [18].

With a slight abuse of terminology, we call $\mathbb{S}^2_X \mathcal{B}$ unit sphere attached at X and, in analogy with the definition of $T\mathcal{B}$, we call bundle of unit spheres the set $\mathbb{S}^2\mathcal{B} = \bigsqcup_{X \in \mathfrak{B}} \mathbb{S}^2_X \mathcal{B}$. When the point $X \in \mathcal{B}$ is not specified, we adopt the notation $\Psi \colon \mathbb{S}^2\mathcal{B} \to \mathbb{R}^+_0$ and $\mathfrak{F} \colon \mathbb{S}^2\mathcal{B} \to \mathbb{R}$, thereby defining both Ψ and \mathfrak{F} over $\mathbb{S}^2\mathcal{B}$. In this case, we introduce the vector field $\boldsymbol{M} \colon \mathcal{B} \to \mathbb{S}^2\mathcal{B}$ such that $\boldsymbol{M}(X) = \boldsymbol{M}_X \in \mathbb{S}^2_X \mathcal{B} \subset \mathbb{S}^2\mathcal{B}$, and we set $\Psi(\boldsymbol{M}(X)) = \Psi_X(\boldsymbol{M}_X)$ and $\mathfrak{F}(\boldsymbol{M}(X)) = \mathfrak{F}_X(\boldsymbol{M}_X)$. Hence, we denote the directional average of \mathfrak{F} by

$$\langle\!\langle \mathfrak{F} \rangle\!\rangle := \int_{\mathbb{S}^2\mathcal{B}} \Psi(M) \mathfrak{F}(M),$$
 (6)

with the understanding that, when $\langle\!\langle \mathfrak{F} \rangle\!\rangle$ is evaluated at $X \in \mathcal{B}$, one obtains $\langle\!\langle \mathfrak{F} \rangle\!\rangle(X) = \langle\!\langle \mathfrak{F}_X \rangle\!\rangle$. Sometimes, since \mathfrak{F} depends on the fibre orientation through the structure tensor, we also use the notation $\langle\!\langle \mathfrak{F}(\mathbf{A}) \rangle\!\rangle = \langle\!\langle \mathfrak{F} \rangle\!\rangle$.

214 2.3 Dynamics

From this point onwards, we employ the symbols "Grad" and "Div" for the gradient and divergence operators in the reference configuration (or, more generally, the body manifold) \mathcal{B} , and the symbols "grad" and "div" for the gradient and divergence operators in the physical space \mathcal{S} . This notation is standard in modern Continuum Mechanics (e.g. [41]) and allows us to be consistent with our previous works, to which we constantly make reference (for some remarks about the notation used in this work, see Appendix A).

We formulate the dynamics of the considered system under the hypoth-222 esis that its constituents (e.g., matrix, fibres, and fluid) have constant mass 223 densities, and no mass exchange processes occur. These assumptions permit 224 to write the mass balance laws of matrix and fibres as $\dot{\Phi}_{0s} = 0$ and $\dot{\Phi}_{1s} = 0$, 225 where the material volumetric fractions $\Phi_{0s} = J\phi_{0s}$ and $\Phi_{1s} = J\phi_{1s}$ are the 226 backward Piola transformations of the spatial volumetric fractions ϕ_{0s} and 227 ϕ_{1s} , respectively. Clearly, Φ_{0s} and Φ_{1s} are independent of time, but they may 228 depend on material points. Moreover, in the material formalism, the balance 229 law of the fluid phase reads 230

$$J + \operatorname{Div} \mathbf{Q} = 0. \tag{7}$$

We recall that our formulation assumes that matrix and fibres undergo the same motion.

Hereafter, we consider the limit of negligible inertial forces and the action of no body forces. Moreover, we assume the validity of Darcy's law. Consistently with this assumption, the Cauchy stress tensor of the fluid phase reduces to $\sigma_{\rm f} = -\phi_{\rm f} p g^{-1}$, where p is called *pore pressure*, and the filtration velocity qis expressed as $q = -k \operatorname{grad} p$, with k being the tissue's permeability tensor. Analogously, the material filtration velocity is given by $\Omega = -K \operatorname{Grad} p$, where $K = J F^{-1} k F^{-T}$ is the material permeability tensor.

The employment of Darcy's law allows to consider only one momentum 240 balance law for the medium as a whole. By introducing the Cauchy stress 241 tensor of the solid phase, $\sigma_{\rm s} = -\phi_{\rm s} p \, g^{-1} + \sigma_{\rm sc}$, where $\sigma_{\rm sc}$ is said to be the 242 constitutive part of $\sigma_{\rm s}$, and since the system is assumed to be closed with 243 respect to momentum, the momentum balance law reads div $\sigma = 0$, where 244 $\sigma \equiv \sigma_{\rm f} + \sigma_{\rm s}$ is the overall Cauchy stress tensor of the medium in the limit 245 of negligibly small relative velocity $w = v_{\rm f} - v_{\rm s}$. To express the balance of 246 momentum in material formalism, we introduce the first Piola-Kirchhoff stress 247 tensors of the fluid phase and of the solid phase, i.e., $P_{\rm f} = J \sigma_{\rm f} F^{-T}$ and 248 $\boldsymbol{P}_{\mathrm{s}} = J\boldsymbol{\sigma}_{\mathrm{s}}\boldsymbol{F}^{-\mathrm{T}}$, respectively, and we obtain 249

$$\operatorname{Div}\left(-Jp\boldsymbol{g}^{-1}\boldsymbol{F}^{-\mathrm{T}}+\boldsymbol{P}_{\mathrm{sc}}\right)=\boldsymbol{0},\tag{8}$$

 $_{250}$ $\,$ where the term between parentheses is the overall first Piola-Kirchhoff stress

tensor of the system, i.e., the sum of $P_{\rm f}$ and $P_{\rm s}$, and $P_{\rm sc} = J\sigma_{\rm sc}F^{-T}$ is the constitutive part of $P_{\rm s}$.

Equations (7) and (8) model the deformation of hydrated soft tissues and 253 the flow of their interstitial fluids, but they cannot describe the dynamics of the 254 internal structure of such tissues. These dynamics, indeed, involve also other 255 processes, which generally occur at different time and length scales, and have 256 distinct biological features. Typical examples of these processes are given by 257 growth, resorption, damage, and reorientation of the network of collagen fibres. 258 A more detailed tissue model should thus consider all these processes and the 259 interactions among them. Nevertheless, we assume here that it is possible to 260 select a modelling range in which one of the aforementioned phenomena can 261 be studied independently of the other ones, at least conceptually [39]. On the 262 basis of this assumption, we propose a theoretical setting in which, besides 263 deformation and fluid flow, we account for the reorientation of fibres in a 264 fibre-reinforced tissue. Moreover, although we present a mathematical model 265 originally conceived for articular cartilage, our results can be extended also to 266 other fibre-reinforced tissues. 267

We claim that remodelling manifests itself through an evolution in time 268 of the mean angle, Q, which has been introduced in the probability density 269 defined in (5a) and (5b). Thus, we call Q remodelling variable from here on. 270 Also ω could be taken as a remodelling variable. However, as done in [39], we 271 prefer here to keep the theory as simple as possible. Thus, we choose ω as a 272 prescribed function of the material points. The remodelling angle Q, instead, 273 evolves starting either from a histological distribution or from a "test" distri-274 bution. In the latter case, one aims to see under which conditions the system 275 remodels towards histological patterns. To emphasise that the probability den-276 sity depends on time through Q (which is now viewed as a function of time 277 and material points), we re-define γ_X and $\bar{\wp}_X$ [cf. (5a) and (5b)] as follows: 278

$$\bar{\wp}_X(\Theta) = \hat{\wp}(\Theta, X, t) = \frac{\gamma_X(\Theta, X, t)}{2\pi \int_0^{\pi/2} \gamma_X(\Theta', X, t) \sin(\Theta') \mathrm{d}\Theta'},$$
(9a)

$$\gamma_X(\Theta) = \hat{\gamma}(\Theta, X, t) = \exp\left(-\frac{\left[\Theta - Q(X, t)\right]^2}{2\left[\omega(X)\right]^2}\right).$$
(9b)

Equations (9a) and (9b) imply that also the probability density Ψ_X depends on time through Q and, consequently, the directional average $\langle\!\langle \mathfrak{F}_X \rangle\!\rangle$ must be regarded as a functional of the remodelling variable, Q. To highlight this dependence, we use the notation $\langle\!\langle \mathfrak{F}_X \rangle\!\rangle \equiv \langle\!\langle \mathfrak{F}_X \rangle\!\rangle (Q)$ from here on.

We remark that the picture of remodelling discussed here and in [22,39] 283 features some similarities with the framework presented Baaijens et al. [42], 284 of which we were unfortunately unaware at the time we wrote the papers 285 [22, 39]. Thus, we take the occasion of this work to state that a description of 286 remodelling based on the evolution of the mean angle characterising the fibres' 287 pseudo-Gaussian probability density can also be found in [42] (cf. Equation 288 (20) of [42]). However, the approach proposed in [22], subsequently developed 289 in [39], and further extended in our work, differs from the one presented in [42] 290 due to the different definition of the generalised forces that drive remodelling, 291

and due to the different methodological framework within which the theory ofremodelling is established.

Following the theory outlined in [19], and subsequently adopted in [27,23], 294 we embrace the line thought according to which the structural evolution of 295 a tissue calls for the introduction of suitable "structural descriptors". These 296 add themselves to the descriptors associated with the standard kinematics of a 297 tissue, namely the velocities of the solid and the fluid phase (or, alternatively, 298 the velocity of the solid phase, $v_{\rm s}$, and the velocity w of the fluid relative to 299 the solid). Within the present framework, we identify the tissue's structural 300 descriptor with the time derivative of the remodelling variable, \dot{Q} , and we call 301 "remodelling forces" the mechanical entities power-conjugate to \dot{Q} [19,27,23]. 302 We distinguish these forces into "internal" and "external", we denote them 303 \mathcal{R}_{int} and \mathcal{R}_{ext} , respectively, and we postulate the force balance [27, 22, 23] 304

$$\mathcal{R}_{\rm int} = \mathcal{R}_{\rm ext}.\tag{10}$$

In conclusion, our theory of remodelling is based on the set of equations (7), (8) and (10), along with (the material counterpart of) Darcy's law $\mathbf{Q} = -\mathbf{K}$ Grad p. We emphasise that we are not regarding Q as an internal variable. Rather, Q is a kinematic variable, having the same "dignity" as the solid phase motion χ , and being determined by solving the balance law (10) associated with it.

Remodelling and deformation couple with each other and, together with 311 fluid flow, drive the overall evolution of the tissue. Such evolution is known 312 after the set of equations (7), (8), and (10) is solved, and the motion χ , pressure 313 p, and remodelling variable Q are determined. To this end, the *remodelling* 314 equation (10) must be rewritten in such a way that it is explicitly solvable for 315 Q. This, in fact, requires to find admissible constitutive laws for the generalised 316 force \mathcal{R}_{int} . To check for thermodynamic admissibility, we exploit the dissipation 317 inequality. 318

We remark that, since our remodelling variable is a scalar parameter, nonplanar remodelling directions cannot be taken into account by our theory. Our choice, however, is meant to keep our model as simple as possible. The model, indeed, can be generalised by introducing two independent remodelling angles, having the meaning of co-latitude and longitude, respectively, and being sufficient to determine univocally the unit vector along which the fibres tend to be aligned.

326 **3 Constitutive theory**

To close the mathematical model, constitutive laws for K and $P_{\rm sc}$ must be supplied. Moreover, whereas the functional form of $\mathcal{R}_{\rm ext}$ has to be prescribed from the outset, $\mathcal{R}_{\rm int}$ must be determined constitutively. In order to do that, a suitable constitutive theory has to be formulated.

331 3.1 Permeability tensor

Following [43], the permeability tensor of a fibre-reinforced porous medium can be determined by invoking the Representation Theorem for functions valued in the space of symmetric second-order tensors [44,45]. Here, we consider the results presented in [43] for the case of a medium exhibiting transverse isotropy with respect to M and, in particular, for the permeability tensor associated with the single fibre, we take the simple expression

$$\boldsymbol{k}_{\text{fibre}} = k_0 \boldsymbol{g}^{-1} + J^{-2} k_0 \boldsymbol{a}, \tag{11}$$

³³⁸ where k_0 is the scalar permeability of the matrix, and a is defined by

$$\boldsymbol{a} = \frac{1}{I_4} \boldsymbol{F} \boldsymbol{A} \boldsymbol{F}^{\mathrm{T}}, \qquad (12)$$

where $I_4 \equiv I_4(\mathbf{C}, \mathbf{A}) = \mathbf{C} : \mathbf{A}$ is the fourth invariant of \mathbf{C} . Note that the original model of Ateshian and Weiss [43] is expressed in terms of the pushforward $\mathbf{F}\mathbf{A}\mathbf{F}^{\mathrm{T}}$ of the material structure tensor \mathbf{A} , whereas (11) features the normalised spatial structure tensor \mathbf{a} . In (11), we assume for k_0 the Holmes and Mow constitutive law [46]

$$k_0 = \hat{k}_0(J) = k_{0R} \left[\frac{J - \Phi_s}{1 - \Phi_s} \right]^{\kappa_0} \exp\left(\frac{1}{2}m_0[J^2 - 1]\right),$$
(13)

where k_{0R} , κ_0 , and m_0 are model parameters. Note that k_{fibre} is a function of F and A, i.e., $k_{fibre} = \hat{k}_{fibre}(F, A)$. Moreover, the spatial permeability of the

tissue, k, is obtained by computing the directional average of k_{fibre} , i.e.,

$$\boldsymbol{k} = \boldsymbol{\hat{k}}(\boldsymbol{F}, \boldsymbol{Q}) = \langle\!\langle \boldsymbol{\hat{k}}_{\text{fibre}}(\boldsymbol{F}, \boldsymbol{A}) \rangle\!\rangle (\boldsymbol{Q}) = \hat{k}_0(J) \boldsymbol{g}^{-1} + J^{-2} \hat{k}_0(J) \boldsymbol{F} \boldsymbol{\hat{Z}}(\boldsymbol{C}, \boldsymbol{Q}) \boldsymbol{F}^{\text{T}},$$
(14)

347 where we introduced the notation

$$\hat{\boldsymbol{Z}}(\boldsymbol{C}, \boldsymbol{Q}) = \left\langle\!\!\left\langle \frac{\boldsymbol{A}}{I_4(\boldsymbol{C}, \boldsymbol{A})} \right\rangle\!\!\right\rangle(\boldsymbol{Q}).$$
(15)

Finally, the material permeability $K = JF^{-1}kF^{-T}$ takes on the form

$$\boldsymbol{K} = \hat{\boldsymbol{K}}(\boldsymbol{C}, Q) = J\hat{k}_0(J)\boldsymbol{C}^{-1} + J^{-1}\hat{k}_0(J)\hat{\boldsymbol{Z}}(\boldsymbol{C}, Q).$$
(16)

349 3.2 Free energy density

³⁵⁰ Our constitutive theory relies on the assumption that the tissue can be asso-

 $_{351}$ ciated with a free energy density consisting of the sum of two contributions,

352 i.e.,

$$W := W_{\rm std} + W_{\rm rem}.\tag{17}$$

1

The first summand, $W_{\rm std}$, is the strain energy density introduced in [16] to model a transversely isotropic biphasic medium with statistical orientation of the fibres. The subscript "std" means that it is regarded as *standard* in the present framework. We write explicitly the expression of $W_{\rm std}$ with the purpose of highlighting its dependence on the remodelling variable:

$$W_{\rm std} = \hat{W}_{\rm std}(\boldsymbol{C}, Q) = \Phi_{\rm s} \hat{U}(J(\boldsymbol{C})) + \Phi_{0\rm s} \hat{W}_{0}(\boldsymbol{C}) + \Phi_{1\rm s} \hat{W}_{\rm e}(\boldsymbol{C}, Q).$$
(18)

Here, Φ_{0s} and Φ_{1s} are the volumetric fractions of matrix and fibres in the reference configuration, respectively, while $\Phi_{s} = \Phi_{0s} + \Phi_{1s}$ is the volumetric fraction of the solid phase as a whole in the same configuration. The term $\hat{U}(J(\mathbf{C}))$ is a penalty enforcing the intrinsic incompressibility of the solid phase at compaction [16], $\hat{W}_{0}(\mathbf{C})$ is the isotropic strain energy density of the matrix, and $\hat{W}_{e}(\mathbf{C}, Q)$ is referred to as "ensemble potential" [14], and constitutes the anisotropic contribution to W_{std} , i.e.,

$$\hat{W}_{\mathrm{e}}(\boldsymbol{C}, Q) = \hat{W}_{\mathrm{1i}}(\boldsymbol{C}) + \langle\!\langle \hat{W}_{\mathrm{1a}}(\boldsymbol{C}, \boldsymbol{A}) \rangle\!\rangle(Q).$$
(19)

The energy densities $\hat{U}(J(\mathbf{C}))$, $\hat{W}_0(\mathbf{C})$, $\hat{W}_{1i}(\mathbf{C})$, and $\hat{W}_{1a}(\mathbf{C}, \mathbf{A})$ are given by

$$\hat{U}(J) = \alpha_0 \mathcal{H}(J_{\rm cr} - J)[J - J_{\rm cr}]^{2q}[J - \Phi_{\rm s}]^{-r}, \qquad (20a)$$

$$\hat{W}_0(\boldsymbol{C}) = \hat{W}_{1i}(\boldsymbol{C}) = \alpha_0 \frac{\exp\left(\alpha_1 [I_1 - 3] + \alpha_2 [I_2 - 3]\right)}{[I_3]^{\alpha_3}},$$
(20b)

$$\hat{W}_{1a}(\boldsymbol{C}, \boldsymbol{A}) = \mathcal{H}(I_4 - 1)\frac{1}{2}c[I_4 - 1]^2,$$
 (20c)

where \mathcal{H} is the Heaviside function (here, $\mathcal{H}(s) = 0$ for all $s \leq 0$, and $\mathcal{H}(s) =$ 366 1 for all s > 0 [38], and we used the short-hand notation $J = J(\mathbf{F}) =$ 367 det \boldsymbol{F} for the volume ratio, $I_1 = I_1(\boldsymbol{C}) = \operatorname{tr}(\boldsymbol{C}), I_2 = I_2(\boldsymbol{C}) = \frac{1}{2} \{ [\operatorname{tr}(\boldsymbol{C})]^2 -$ 368 $\operatorname{tr}(\mathbf{C}^2)$, $I_3 = I_3(\mathbf{C}) = \det \mathbf{C}$ for the three principal invariants of \mathbf{C} , and 369 $I_4 = I_4(\boldsymbol{C}, \boldsymbol{A}) = \boldsymbol{C} : \boldsymbol{A}$ for the fourth invariant of \boldsymbol{C} . In (20a), $J_{\rm cr} \in [\Phi_{\rm s}, 1]$ 370 is a "critical" value of J below which the penalty term is switched on to 371 prevent J from approaching the lower physical bound Φ_s , while $q \geq 2$ and 372 $r \in [0,1]$ are model parameters. In (20b) and (20c), α_0 , α_1 , α_2 , α_3 , and c are 373 model parameters and, in particular, α_0 and c have the same physical units 374 as the strain energy density and determine the energy scales characterising 375 the isotropic and anisotropic contributions of $W_{\rm std}$. The term $W_{\rm 1i}(C)$ is the 376 isotropic contribution of the fibres to the tissue's overall strain energy density, 377 and $W_{1a}(C, A)$ is the anisotropic contribution, which depends on the fibre 378 alignment through $A = M \otimes M$. The fact that \hat{W}_{1i} is taken here to be 379 equal to \hat{W}_0 is just a model assumption [38]. We remark that the directional 380 average of $\hat{W}_{1a}(\boldsymbol{C}, \boldsymbol{A})$, i.e., $\langle\!\langle \hat{W}_{1a}(\boldsymbol{C}, \boldsymbol{A}) \rangle\!\rangle$, depends on the remodelling variable, 381 Q, through the probability density. 382

The idea underlying the definition of the energy density given in (18) can be found in several works on composite materials [47–49]. In these papers, a given composite material is modelled within the theory of linear elasticity, and the elasticity tensor of the material is written as the weighted sum of the elasticity tensors of its constituents, each multiplied by the corresponding

volumetric fraction. In this sum, however, the weights depend on the strain 388 concentration tensor [49,50] and, thus, on Eshelby's fourth-order tensor [51]. 389 In the non-linear framework, instead, the Eshelby-like formulation is not di-390 rectly applicable and, if the constituents of a composite material are assumed 391 to be hyperelastic, the elastic potential of the composite as a whole can be con-392 structed by weighing the elastic potentials of the constituents. In some cases, 393 e.g. [2,27], the elastic potentials contain the volumetric fractions in their own 394 definition, whereas we put them in evidence in our formulation. In (18), in-395 deed, apart from $\Phi_{\rm s} \hat{U}(J(\mathbf{C}))$, $W_{\rm std}$ is the weighted sum of one contribution 396 due to the matrix and one due to the fibres, the weights being the volumetric 397 fractions Φ_{0s} and Φ_{1s} . 398

Moreover, in the present work, the isotropic energy densities $\hat{W}_0(C)$ and 300 $\hat{W}_{1i}(C)$ depend on I_3 , thereby describing a compressible behaviour of the 400 modelled material, while the anisotropic contribution, $\hat{W}_{1a}(C, A)$, is assumed 401 to depend on C through I_4 only. In fact, the tissue described by (18), (19), 402 and (20a)–(20c) is compressible and anisotropic, which requires its elastic en-403 ergy density to depend both on I_3 and —at least— on I_4 . However, the way 404 in which compressibility and anisotropy are modelled is not unique and, in 405 this respect, the additive decomposition of the energy density performed in 406 (18) and (19), in which the compressible effects are attributed solely to the 407 isotropic terms, is only one among other possible choices. To give an example, 408 indeed, in the work by Almeida and Spilker [52] on articular cartilage, the 409 elastic energy density is anisotropic and compressible, but the decomposition 410 presented in (18) and (19) was not enforced. We would like to emphasise, 411 however, that decompositions of this kind are rather customary in the study 412 of fibre-reinforced hyperelastic materials (see e.g. [2,27] for the case of blood 413 vessels). Moreover, strictly speaking, since I_4 can be further decomposed mul-414 tiplicatively as $I_4 = I_3^{1/3} \bar{I}_4$, with $\bar{I}_4 = \bar{C} : A$ and det $\bar{C} = 1$, the anisotropic 415 part of the energy density still models a compressible material. 416

⁴¹⁷ The second summand of (17), W_{rem} , is the part of the free energy density ⁴¹⁸ that is directly related to remodelling. This term is the main novelty of our ⁴¹⁹ constitutive theory, which is based on the requirement that W_{rem} admits the ⁴²⁰ representation

$$W_{\rm rem} = \hat{W}_{\rm rem}(\boldsymbol{C}, \boldsymbol{Q}, \operatorname{Grad} \boldsymbol{Q}) = \hat{W}_{\rm str}(\boldsymbol{C}, \boldsymbol{Q}) + \hat{W}_{\rm grad}(\boldsymbol{C}, \operatorname{Grad} \boldsymbol{Q}).$$
(21)

421 The energy densities $\hat{W}_{\text{grad}}(\boldsymbol{C}, \operatorname{Grad} Q)$ and $\hat{W}_{\text{str}}(\boldsymbol{C}, Q)$ are given by

 $W_{\text{grad}} = \hat{W}_{\text{grad}}(\boldsymbol{C}, \operatorname{Grad} Q) = \frac{1}{2} \hat{\boldsymbol{D}}(\boldsymbol{C}) : \operatorname{Grad} Q \otimes \operatorname{Grad} Q,$ (22a)

$$W_{\rm str} = \hat{W}_{\rm str}(\boldsymbol{C}, Q) = \hat{\mathcal{A}}(\boldsymbol{C})\hat{\mathcal{P}}(Q)\exp\left(\hat{\alpha}_W(\boldsymbol{C})Q\right),\tag{22b}$$

where the subscript "grad" indicates that \hat{W}_{grad} depends on the gradient of the mean angle, while the subscript "str" means that \hat{W}_{str} is directly related to the internal structure of the tissue. The quantity $\hat{D}(C)$ is a symmetric, positive semi-definite, second-order tensor-valued function of C, $\hat{A}(C)$ is a non-negative coefficient with physical units of energy per unit volume, $\hat{\mathcal{P}}(Q)$ is a dimensionless, non-negative function of Q, and $\hat{\alpha}_W(C)$ is a dimensionless, non-negative coefficient. In the absence of deformation, i.e., when C equals the material metric tensor G (which serves here as the "covariant identity tensor"), we set $\hat{D}(G) = D_0$, $\hat{A}(C) = A_0 \ge 0$, and $\hat{\alpha}_W(G) = 0$.

The term $W_{\text{grad}}(\boldsymbol{C}, \text{Grad } Q)$ is introduced to explicitly account for the 431 spatial resolution of the remodelling variable, Q. Physically, it represents the 432 contribution to the overall energy that is set off by the first-order spatial 433 variations of Q at each material point. To keep the proposed theory at a 434 minimal level of complexity, we assume that $\hat{W}_{\text{grad}}(\boldsymbol{C}, \text{Grad } Q)$ is quadratic in 435 $\operatorname{Grad} Q$. As is the case for other theories based on energy densities that depend 436 on the gradient of an angular variable (for example, the energy of the Sine-437 Gordon model [53]), $\hat{D}(C)$ could be thought of as a measure of the system's 438 "angular stiffness per unit length". Indeed, it determines the response of the 439 system to the spatial variations of Q. We remark that, by its own definition, 440 D(C) is modulated by C, which means that, in general, the tissue's angular 441 stiffness varies with the deformation. If, on the one hand, the evolution of 442 the remodelling angle Q influences the elastic response of the tissue through 443 the term $\hat{W}_{e}(C,Q)$ [see Equation (18)], the tensor $\hat{D}(C)$ couples the global 444 changes of shape of the tissue with its structural transformations, which are 445 represented by the variations of Q in time and space. 446

Before providing a term-by-term explanation of $W_{\rm str}(C,Q)$ [see (22b)], we 447 discuss the logical steps that lead to its functional form. First, we remark that, 448 since in this work the kinematics of the tissue is described by χ and Q, the 449 configuration attained by the tissue at time t is determined by both $\chi(X,t)$ 450 and Q(X,t), for all $X \in \mathcal{B}$. Second, we claim that each such configuration 451 can be associated with an energy that depends on the deformation and the 452 distribution of the fibre mean angle throughout the tissue. Third, by exploiting 453 the fact that the deformation and the mean angle are independent on each 454 other, we also claim that there exist distributions of the fibre mean angle that 455 endow the tissue with non-trivial energies even in the absence of deformation. 456 Indeed, even though $W_{\rm std}$ reduces to the unessential constant $\hat{W}_{\rm std}(\boldsymbol{G}, \boldsymbol{Q}) \equiv$ 457 $\hat{W}_{\text{std}}^{(0)}(Q) = \alpha_0$ in such cases [see (18) and (20a)–(20c)], W_{str} and W_{grad} become 458

$$\hat{W}_{\rm str}(\boldsymbol{G}, Q) \equiv \hat{W}_{\rm str}^{(0)}(Q) = \mathcal{A}_0 \hat{\mathcal{P}}(Q), \qquad (23a)$$

$$\hat{W}_{\text{grad}}(\boldsymbol{G}, \operatorname{Grad} Q) \equiv \hat{W}_{\text{grad}}^{(0)}(\operatorname{Grad} Q) = \frac{1}{2}\boldsymbol{D}_0 : \operatorname{Grad} Q \otimes \operatorname{Grad} Q, \quad (23b)$$

459 thereby yielding

$$W_{\text{rem}} \equiv \hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad}\,Q) = \hat{W}_{\text{str}}^{(0)}(Q) + \hat{W}_{\text{grad}}^{(0)}(\text{Grad}\,Q),$$

$$= \mathcal{A}_0 \hat{\mathcal{P}}(Q) + \frac{1}{2} \boldsymbol{D}_0 : \text{Grad}\,Q \otimes \text{Grad}\,Q, \qquad (24a)$$

$$W \equiv \hat{W}_{\text{std}}^{(0)}(Q) + \hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad}\,Q)$$

$$= \alpha_0 + \hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad}\,Q).$$
(24b)

If D_0 is positive definite and \mathcal{A}_0 strictly positive, $\hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad }Q)$ is zero only for those distributions of the fibre mean angle that are spatially uniform

and solutions of $\hat{\mathcal{P}}(Q) = 0$. In the jargon of [53], a time-independent field Q 462 satisfying these conditions is said to be a "classical vacuum" configuration for 463 $\hat{W}^{(0)}_{\rm rem}(Q, \operatorname{Grad} Q)$, since it determines the lowest energy of the system under 464 study (zero, in the considered case). In general, however, when Q is not a 465 vacuum configuration, $\hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad } Q)$ is greater than zero and consists of 466 the contribution due to the spatial variability of Q, i.e., $\hat{W}_{\text{grad}}^{(0)}(\text{Grad }Q)$, and of the contribution due to the potential energy density associated with Q, i.e., $\hat{W}_{\text{str}}^{(0)}(\text{Grad }Q)$. Thus, up to α_0 , $\hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad }Q)$ is the energy density that 467 468 469 characterises the tissue for a given Q, and the integral 470

$$\mathcal{W}_{\text{rem}}^{(0)}[Q] = \int_{\mathcal{B}} \hat{W}_{\text{rem}}^{(0)}(Q, \operatorname{Grad} Q)$$
$$= \int_{\mathcal{B}} \left\{ \mathcal{A}_0 \hat{\mathcal{P}}(Q) + \frac{1}{2} \boldsymbol{D}_0 : \operatorname{Grad} Q \otimes \operatorname{Grad} Q \right\}$$
(25)

⁴⁷¹ is the tissue's energy corresponding to Q. In conclusion, and consistently with
⁴⁷² what we claimed above, our interpretation of (25) is that any conformation of
⁴⁷³ the tissue's internal structure, which is described by selecting an appropriate
⁴⁷⁴ distribution of the fibre mean angle, yields an energy. This energy, in turn, is
⁴⁷⁵ nonzero as long as the distribution of the fibre mean angle is not a vacuum
⁴⁷⁶ configuration.

As explained in Section 4.1, we assume that the information on the internal 477 structure of the tissue is supplied by the histological pattern with which the 478 fibres are oriented in the undeformed tissue and, thus, by the distribution of 479 the fibre mean angle associated with it. Such distribution, denoted by $Q_{\rm h}$, 480 can be determined experimentally. In fact, as shown in Fig. 2, it features a 481 sigmoidal shape and takes on the values $Q_0 = 0$ rad and $Q_1 = \pi/2$ rad at the 482 lower and upper boundary, respectively, of the cylindrical samples of tissue 483 adopted in the study [54]. 484

Although a functional form for $Q_{\rm h}$ can be obtained by fitting experimental data [54], we follow here a rather different approach. First, since the sigmoidal profile of $Q_{\rm h}$ goes from Q_0 to Q_1 , we invoke a formal analogy with the theory of phase transitions, and we claim that $\hat{W}_{\rm str}^{(0)}(Q)$ should be a double-well energy density of the Allen-Cahn type, with $Q_0 = 0$ rad and $Q_1 = \pi/2$ rad being its global minimum configurations. Thus, with reference to the undeformed configuration of the tissue, we set

$$\hat{W}_{\rm str}^{(0)}(Q) \equiv \hat{W}_{\rm AC}^{(0)}(Q) = \frac{\mathcal{A}_0}{(\pi/4)^4} Q^2 \left(Q - \frac{\pi}{2}\right)^2,\tag{26}$$

where $\hat{W}^{(0)}_{AC}(Q)$ is the Allen-Cahn energy density [26]. We notice that Equations (23a) and (26) allow to identify $\hat{\mathcal{P}}(Q)$ with

$$\hat{\mathcal{P}}(Q) = \frac{1}{(\pi/4)^4} Q^2 \left(Q - \frac{\pi}{2}\right)^2,$$
(27)

⁴⁹⁴ i.e., with a polynomial of degree four in Q that vanishes for $Q_0 = 0$ rad and ⁴⁹⁵ $Q_1 = \pi/2$ rad, and whose global maximum over $[0, \pi/2]$ is attained at $Q_{\text{max}} =$ ⁴⁹⁶ $\pi/4$ rad.

We emphasise that the zeroes of $\hat{\mathcal{P}}(Q)$ are the vacuum configurations of the Allen-Cahn energy density defined in Equation (26), for which it holds, thus, $\hat{W}_{AC}^{(0)}(Q_0) = \hat{W}_{AC}^{(0)}(Q_1) = 0$. Accordingly, the sigmoidal profile of Q_h describes a transition from Q_0 to Q_1 , and the quantity \mathcal{A}_0 , which is equal to the global maximum of $\hat{W}_{AC}^{(0)}(Q)$, defines the height of the energy barrier separating Q_0 from Q_1 .

⁵⁰³ When the deformation is considered, the height of the energy barrier, \mathcal{A}_0 , ⁵⁰⁴ is generally allowed to be modulated by the deformation, and becomes $\hat{\mathcal{A}}(\boldsymbol{C})$. ⁵⁰⁵ Moreover, whereas $\hat{W}_{AC}^{(0)}(Q)$ is symmetric with respect to $Q = \pi/4$ rad, the ⁵⁰⁶ coefficient $\hat{\alpha}_W(\boldsymbol{C})$ destroys this symmetry for $\boldsymbol{C} \neq \boldsymbol{G}$. In conclusion, by using ⁵⁰⁷ the expression of $\hat{\mathcal{P}}(Q)$ given in (27), we can interpret the structural part ⁵⁰⁸ of the energy density, $\hat{W}_{str}(\boldsymbol{C}, Q)$, as a generalised, deformation-dependent ⁵⁰⁹ energy density of the Allen-Cahn type, i.e.,

$$\hat{W}_{\rm AC}(\boldsymbol{C}, Q) \equiv \hat{W}_{\rm str}(\boldsymbol{C}, Q) = \hat{\mathcal{A}}(\boldsymbol{C})\hat{\mathcal{P}}(Q)\exp(\hat{\alpha}_W(\boldsymbol{C})Q).$$
(28)

Although all the results presented in this work have been obtained by employing $\hat{W}_{AC}^{(0)}(Q)$ and $\hat{W}_{AC}(C,Q)$, these energy densities may have to be replaced with more appropriate constitutive choices in the case of different histological distributions of the mean angle, or for tissues other than articular cartilage. However, if the spatial resolution of the mean angle has to be explicitly taken into account, a "gradient-part" of the remodelling energy, like the one defined in (22a), may still be employed.

Once the Allen-Cahn energy density (28) is introduced, we claim that Q_h can be determined as the solution of a variational problem. To this end, indeed, we require that the first-order variation of the functional $\mathcal{W}_{rem}^{(0)}$, defined in (25), is zero for arbitrary variations of Q_h .

In Section 4.1 it will be shown that $Q_{\rm h}$ is computed by solving a differential 521 equation equipped with the Dirichlet boundary conditions $Q_{\rm h}(X) = Q_0$, for 522 all $X \in (\partial \mathcal{B})_{L}$, and $Q_{h}(X) = Q_{1}$, for all $X \in (\partial \mathcal{B})_{U}$, where $(\partial \mathcal{B})_{L}$ and $(\partial \mathcal{B})_{U}$ 523 denote the lower and upper boundaries of B, respectively. In this case, the 524 magnitude of D_0 influences the tendency of the fibre mean angle to become a 525 straight line connecting Q_0 with Q_1 . This trend, in fact, is obtained in the limit 526 in which the magnitude of D_0 goes towards infinity. On the other hand, if the 527 boundary data are changed in such a way that one of the two Dirichlet condi-528 tions is replaced by a homogeneous Neumann condition, then the magnitude 529 of D_0 measures the tendency of Q_h to distribute itself uniformly throughout 530 the sample. When this is the case, indeed, the uniformity of $Q_{\rm h}$ increases with 531 the magnitude of D_0 . Finally, when the deformation is considered, and the 532 evolution in time of the fibre mean angle, Q, is studied, D(C) influences the 533 rate at which Q approaches a stationary solution. 534

535 3.3 Dissipation Inequality

- ⁵³⁶ In the present context, the dissipation inequality can be cast in the form [22]
- 537 (see Appendix B for details)

$$\mathfrak{D} = \mathfrak{D}_{\mathrm{I}} + \mathfrak{D}_{\mathrm{II}} + \mathfrak{D}_{\mathrm{IV}} \ge 0, \tag{29}$$

- where \mathfrak{D} is the residual dissipation per unit volume of the reference configu-
- ration, and the summands on the right-hand-side of (29) are given by

$$\mathfrak{D}_{\mathrm{I}} = \left\{ -F\left(2\frac{\partial\hat{W}}{\partial C}\right) + P_{\mathrm{s}} + \Phi_{\mathrm{s}}p\,\boldsymbol{g}^{-1}F^{-\mathrm{T}} \right\} : \boldsymbol{g}\dot{F} + \left\{ P_{\mathrm{f}} + (J - \Phi_{\mathrm{s}})p\,\boldsymbol{g}^{-1}F^{-\mathrm{T}} \right\} : \boldsymbol{g}\,\mathrm{Grad}\boldsymbol{v}_{\mathrm{f}},$$
(30a)

$$\mathfrak{D}_{\mathrm{II}} = -J \left[\boldsymbol{\pi}_{\mathrm{f}} - p \boldsymbol{g}^{-1} \mathrm{grad} \, \boldsymbol{\phi}_{\mathrm{f}} \right] . \boldsymbol{w}, \qquad (30\mathrm{b})$$

$$\mathfrak{D}_{\mathrm{III}} = \left\{ -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(\frac{\partial \hat{W}}{\partial \operatorname{Grad} Q} \right) \right] + \mathfrak{R}_{\mathrm{int}} \right\} \dot{Q}, \quad (30c)$$

$$\mathfrak{D}_{\rm IV} = {\rm Div} \left[-T \bar{\mathfrak{Q}}^{\eta} - \frac{\partial \hat{W}}{\partial {\rm Grad}Q} \dot{Q} \right].$$
(30d)

Here, $\bar{\mathfrak{Q}}^{\eta}$ is the entropy flux vector, and \hat{W} is expressed constitutively as

$$\hat{W}(\boldsymbol{C}, \boldsymbol{Q}, \operatorname{Grad}\boldsymbol{Q}) = \hat{W}_{\operatorname{std}}(\boldsymbol{C}, \boldsymbol{Q}) + \hat{W}_{\operatorname{rem}}(\boldsymbol{C}, \boldsymbol{Q}, \operatorname{Grad}\boldsymbol{Q}),$$
(31a)

$$\hat{W}_{\text{rem}}(\boldsymbol{C}, \boldsymbol{Q}, \text{Grad}\boldsymbol{Q}) = \hat{W}_{\text{AC}}(\boldsymbol{C}, \boldsymbol{Q}) + \frac{1}{2}\hat{\boldsymbol{D}}(\boldsymbol{C}) : \text{Grad}\boldsymbol{Q} \otimes \text{Grad}\boldsymbol{Q}.$$
 (31b)

Also the constitutive part of the mechanical stress depends —at least in 541 principle— on the same list of variables. However, to account for the dissi-542 pation related to the exchange of momentum between the fluid and the solid 543 phase (which is represented by $\mathfrak{D}_{II} \geq 0$, and leads to Darcy's law) as well as 544 for the dissipation associated with remodelling (i.e., $\mathfrak{D}_{III} \geq 0$), the complete 545 list of independent constitutive variables is given by F, Q, Grad Q, \dot{Q} , and 546 w. Furthermore, we study the dissipation inequality (29) by requiring that 547 $\mathfrak{D}_{\mathrm{I}}, \mathfrak{D}_{\mathrm{II}}, \mathfrak{D}_{\mathrm{III}}, \mathrm{and} \mathfrak{D}_{\mathrm{IV}}$ are all non-negative, one independently on the others. 548 Within the present theoretical framework, in which the free energy density 549 \hat{W} features the gradient of the remodelling variable among its arguments, the 550 entropy flux vector does not necessarily reduce to the ratio between a heat 551 flux vector and the absolute temperature [55]. Rather, $\bar{\mathfrak{Q}}^{\eta}$ is defined by 552

$$\bar{\mathfrak{Q}}^{\eta} = -\frac{1}{T} \frac{\partial \hat{W}}{\partial \mathrm{Grad}Q} \dot{Q}, \qquad (32)$$

thereby establishing that \mathfrak{D}_{IV} vanishes identically. Moreover, since \dot{F} and Grad v_f are not independent constitutive variables, and \mathfrak{D}_I depends linearly on them, the sums between braces in (30a) must be zero to ensure that the

16

⁵⁵⁶ inequality $\mathfrak{D}_{\mathrm{I}} \geq 0$ is fulfilled for arbitrary choices of \dot{F} and $\mathrm{Grad}v_{\mathrm{f}}$. Hence, $\mathfrak{D}_{\mathrm{I}}$ ⁵⁵⁷ vanishes identically. This yields the conditions

$$\boldsymbol{P}_{s} = -\boldsymbol{\Phi}_{s} \boldsymbol{p} \boldsymbol{g}^{-1} \boldsymbol{F}^{-T} + \boldsymbol{F} \left(2 \frac{\partial \hat{W}}{\partial \boldsymbol{C}} \right), \qquad (33a)$$

$$\boldsymbol{P}_{\rm f} = -(J - \Phi_{\rm s}) p \, \boldsymbol{g}^{-1} \boldsymbol{F}^{-\rm T}, \tag{33b}$$

$$\boldsymbol{P} = \boldsymbol{P}_{s} + \boldsymbol{P}_{f} = -Jp \,\boldsymbol{g}^{-1} \boldsymbol{F}^{-T} + \boldsymbol{F} \left(2 \frac{\partial W}{\partial \boldsymbol{C}} \right), \qquad (33c)$$

so that the constitutive part $\boldsymbol{P}_{\mathrm{sc}}$ of $\boldsymbol{P}_{\mathrm{s}}$ and \boldsymbol{P} is given by

$$\boldsymbol{P}_{\rm sc} = \boldsymbol{F}\left(2\frac{\partial\hat{W}}{\partial\boldsymbol{C}}\right). \tag{34}$$

Note that, if the free energy density is given as a function of F, Q, and the spatial gradient of Q, i.e., as $\hat{\mathcal{V}}(F, Q, \operatorname{grad} Q) = \hat{W}(C, Q, \operatorname{Grad} Q)$, P_{sc} admits the two equivalent expressions

$$\boldsymbol{P}_{\rm sc} = \boldsymbol{F}\left(2\frac{\partial\hat{W}}{\partial\boldsymbol{C}}\right) = \boldsymbol{g}^{-1}\frac{\partial\hat{V}}{\partial\boldsymbol{F}} + \boldsymbol{P}_{\rm K},\tag{35a}$$

$$\boldsymbol{P}_{\mathrm{K}} = -\boldsymbol{g}^{-1} \left(\operatorname{grad} Q \otimes \frac{\partial \hat{\boldsymbol{\mathcal{V}}}}{\partial \operatorname{grad} Q} \right) \boldsymbol{F}^{-\mathrm{T}}, \tag{35b}$$

where $P_{\rm K}$ is the Piola transform of the Korteweg stress tensor [55]. We em-

⁵⁶³ phasise that the presence of $P_{\rm K}$, which is explicit in (35a) and hidden in (34), ⁵⁶⁴ is a consequence of the fact that our theory employs a free energy density ⁵⁶⁵ depending on Grad Q.

Finally, we define the dissipative generalised forces $\pi_{\rm fd}$ and \mathcal{N} , i.e.,

$$\boldsymbol{\pi}_{\rm fd} \equiv \boldsymbol{\pi}_{\rm f} - p \boldsymbol{g}^{-1} \text{grad} \, \phi_{\rm f}, \tag{36a}$$

$$\mathcal{N} \equiv -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(\frac{\partial \hat{W}}{\partial \operatorname{Grad}Q}\right)\right] + \mathcal{R}_{\operatorname{int}},\tag{36b}$$

567 so that the residual dissipation reads

$$\mathfrak{D} = -J\boldsymbol{\pi}_{\mathrm{fd}}.\boldsymbol{w} + \mathfrak{N}\dot{\boldsymbol{Q}} \ge 0.$$
(37)

⁵⁶⁸ While the first term on the right-hand-side of (37) is rather standard and is ⁵⁶⁹ assumed to lead to Darcy's law in the present framework, the term $N\dot{Q}$ is ⁵⁷⁰ "new", in the sense that it is generated by the presence of remodelling [27, ⁵⁷¹ 22,39]. Since the remodelling equation is given by $\mathcal{R}_{int} = \mathcal{R}_{ext}$, and since ⁵⁷² \mathcal{R}_{int} comprises a dissipative part, \mathcal{N} , as well as a non-dissipative part (which ⁵⁷³ coincides with the terms between brackets in (36b)), we write

$$\mathcal{R}_{int} \equiv \mathcal{N} + \left[\frac{\partial \hat{W}}{\partial Q} - \text{Div} \left(\frac{\partial \hat{W}}{\partial \text{Grad}Q} \right) \right] = \mathcal{R}_{ext}.$$

(38)

574 Hence, we obtain

$$\mathcal{N} = -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(\frac{\partial \hat{W}}{\partial \operatorname{Grad}Q}\right)\right] + \mathcal{R}_{\mathrm{ext}}.$$
(39)

⁵⁷⁵ Following [22,39], we prescribe \mathcal{N} to be defined through a particular simple ⁵⁷⁶ constitutive law that is linear in \dot{Q} , i.e.,

$$\mathcal{N} = \hat{\mathcal{N}}(\boldsymbol{C}, \boldsymbol{Q}, \dot{\boldsymbol{Q}}) = \hat{\boldsymbol{\Gamma}}(\boldsymbol{C}, \boldsymbol{Q})\dot{\boldsymbol{Q}},\tag{40}$$

with $\hat{\Gamma}(\boldsymbol{C}, Q) \geq 0$, so that the remodelling equation becomes

$$\hat{\Gamma}(\boldsymbol{C}, Q) \dot{Q} = -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(\frac{\partial \hat{W}}{\partial \operatorname{Grad}Q}\right)\right] + \mathcal{R}_{\mathrm{ext}}$$
$$= -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(\hat{\boldsymbol{D}}(\boldsymbol{C})\operatorname{Grad}Q\right)\right] + \mathcal{R}_{\mathrm{ext}}.$$
(41)

Equation (41) is the *remodelling equation* that rules the evolution of the remodelling variable Q. With respect to other pictures of remodelling (for instance, those put forward in [27,22,23]), the theory proposed here contains the additional internal remodelling force

$$-\operatorname{Div}\left(\frac{\partial \hat{W}}{\partial \operatorname{Grad}Q}\right) = -\operatorname{Div}\left(\hat{\boldsymbol{D}}(\boldsymbol{C})\operatorname{Grad}Q\right).$$
(42)

We remark that the terms in brackets in (41) are *not* the functional derivative of \hat{W}_{rem} . Indeed, also \hat{W}_{std} depends on Q and, thus, contributes to the evolution of the remodelling variable. Before going further, we mention that similar constitutive frameworks, based however on the Cahn-Hilliard model, have been proposed in studying tumours in [56–58].

⁵⁸⁷ 3.4 Summary of the model equations and simplifying assumptions

The model equations are given by (7), (8), and (41). These have to be solved 588 by providing boundary conditions, as well as initial conditions for χ and Q. In 589 this work, we consider a sample of tissue of cylindrical shape in its reference 590 configuration, B. We denote by L = 1 mm and R = 1.5 mm the initial thickness 591 and initial radius of the sample, respectively, and we write the boundary of \mathcal{B} 592 as the disjoint union $\partial \mathcal{B} = (\partial \mathcal{B})_L \sqcup (\partial \mathcal{B})_U \sqcup (\partial \mathcal{B})_B$, where $(\partial \mathcal{B})_L$, $(\partial \mathcal{B})_U$, and 593 $(\partial \mathcal{B})_{B}$ represent the lower, upper, and lateral portions of $\partial \mathcal{B}$, respectively. The 594 sample is assumed to be transversely isotropic with respect to the direction 595 M_0 , which coincides with the geometric symmetry axis of the cylinder. 596

The sample is subjected to an unconfined compression test characterised by the boundary conditions (BCs)

On
$$(\partial \mathcal{B})_{\mathrm{U}}, \quad \begin{cases} \chi^3 = \mathfrak{g}, \\ (-\boldsymbol{K} \operatorname{Grad} p).\boldsymbol{N} = 0, \end{cases}$$
 (43a)

18

(

On
$$(\partial \mathcal{B})_{\mathrm{L}}$$
,
$$\begin{cases} \chi(X,t) - \chi(X,0) = \mathbf{0}, \\ (-\mathbf{K} \operatorname{Grad} p) \cdot \mathbf{N} = 0, \end{cases}$$
 (43b)

On
$$(\partial \mathcal{B})_{\rm B}$$
,
$$\begin{cases} (-Jp\boldsymbol{g}^{-1}\boldsymbol{F}^{-{\rm T}} + \boldsymbol{P}_{\rm sc}).\boldsymbol{N} = 0,\\ p = 0, \end{cases}$$
(43c)

where χ^3 is the axial component of the solid phase motion, N is the field of unit normal to $\partial \mathcal{B}$, and \mathfrak{g} is the compressive loading history

$$\mathfrak{g}(t) = \begin{cases} L - \frac{t}{T_{\text{ramp}}} u_{\text{T}}, & \text{for } t \in [0, T_{\text{ramp}}], \\ L - u_{\text{T}}, & \text{for } t \in]T_{\text{ramp}}, T_{\text{end}}]. \end{cases}$$
(44)

The target displacement $u_{\rm T} = 0.2 \,\mathrm{mm}$ is reached by $(\partial \mathcal{B})_{\rm U}$ at $T_{\rm ramp} = 20 \,\mathrm{s}$, and then maintained up to $T_{\rm end} = 100 \,\mathrm{s}$. The BCs (43a) and (43b) indicate that $(\partial \mathcal{B})_{\rm U}$ and $(\partial \mathcal{B})_{\rm L}$ are impermeable, with $(\partial \mathcal{B})_{\rm U}$ being displaced axially according to \mathfrak{g} , and $(\partial \mathcal{B})_{\rm L}$ being kept fixed. The BCs (43c), instead, imply that $(\partial \mathcal{B})_{\rm B}$ is permeable and free of applied surface forces. A schematic description of the considered benchmark test is given in Fig. 1.



Fig. 1 Schematic description of the considered loading history. The sample is compressed along the axial direction by means of a loading ramp up to $t \leq T_{\text{ramp}} = 20 \text{ s}$, and the load is then maintained up to $T_{\text{end}} = 100 \text{ s}$.

In addition to (43a)–(43c), we also prescribe the BCs for the remodelling variable, Q, i.e.,

On $(\partial \mathcal{B})_{\mathrm{U}}$, $Q(X,t) = \frac{\pi}{2}$ rad, $\forall t \in]0, T_{\mathrm{end}}]$, (45a)

On
$$(\partial \mathcal{B})_{\mathrm{L}}$$
, $Q(X,t) = 0 \,\mathrm{rad}$, $\forall t \in [0, T_{\mathrm{end}}]$, (45b)

On
$$(\partial \mathcal{B})_{\mathrm{B}}$$
, $(-\hat{\boldsymbol{D}}(\boldsymbol{C}) \operatorname{Grad} \boldsymbol{Q}) \cdot \boldsymbol{N} = 0$, $\forall t \in]0, T_{\mathrm{end}}]$ (45c)

Finally, the initial condition on χ is expressed by requiring that the reference configuration, which coincides here with the initial one, is undeformed, while the initial condition on Q can be either obtained by fitting experimental data or computed via preliminary calculations, as explained in Section 4.1.

We remark that the boundary conditions imposed on *Q* are necessary to solve the partial differential equation governing its spatiotemporal evolution. Among various possible choices (i.e., boundary conditions of Dirichlet, Neumann, or mixed type), we chose Dirichlet boundary conditions because they

are easier to handle from a numerical point of view, and because they are 617 consistent with the histological information on the pattern of fibre alignment 618 within the tissue. Clearly, imposing these conditions on the upper and lower 619 boundary of the sample prescribes the values of the remodelling variable on 620 these surfaces. This, in turn, amounts to restrict the remodelling process only 621 to the internal points of the sample, and, in the case studied in Section 4.1, 622 guides the distribution of the fibre mean angle towards the expected result. 623 However, this requirement seems to us weaker, and therefore more general, 624 than prescribing the histological profile a priori, or selecting an ad hoc remod-625 elling force \mathcal{R}_{ext} . Moreover, the use of boundary conditions of different type, 626 and their impact on the solution describing the distribution of the fibre mean 627 angle is part of our current investigations. 628

Before going further, it is important to analyse the explicit expression of $2(\partial \hat{W}/\partial C)$ and $\partial \hat{W}/\partial Q$. For this purpose, we invoke the constitutive laws (18)-(26), (31a) and (31b), and we enforce the simplifying assumptions $\hat{\mathcal{A}}(C) =$ $\mathcal{A}_0, \hat{D}(C) = D_0 G^{-1}$ (the inverse metric G^{-1} here serves as the "contravariant identity tensor"), and $\hat{\Gamma}(C, Q) = \Gamma$, where \mathcal{A}_0, D_0 , and Γ are assumed to be constant. Moreover, we set

$$\hat{\alpha}_W(\mathbf{C}) = \frac{1}{2}a[I_1(\bar{\mathbf{C}}) - 3]^2,$$
(46)

with a being a non-negative scalar constant, and $\bar{C} = J^{-2/3}C$. We need to 635 clarify, however, that, since D_0 and \mathcal{A}_0 must vanish in the absence of fibres, 636 both D_0 and \mathcal{A}_0 should be expressed by means of continuous functions of the 637 volumetric fraction of the fibres, Φ_{1s} , that tend to zero when Φ_{1s} tends to zero. 638 Furthermore, since Φ_{1s} is a function of the material point, D_0 and \mathcal{A}_0 should 639 depend on the material point too. Therefore, the assumption of constant D_0 640 and \mathcal{A}_0 means that these coefficients correspond to averaged values of Φ_{1s} . In 641 the cases in which this hypothesis in invalid, D_0 and A_0 should be reformulated 642 as $D_0 = \Phi_{1s}\tilde{D}_0$ and $\mathcal{A}_0 = \Phi_{1s}\tilde{\mathcal{A}}_0$, where $\tilde{D}_0 \ge 0$ and $\mathcal{A}_0 \ge 0$ may also depend 643 on the material point, in general. 644

The assumptions done so far imply that the free energy density used for simulations is given by

$$\hat{W}(\boldsymbol{C}, \boldsymbol{Q}, \operatorname{Grad}\boldsymbol{Q}) = \hat{W}_{\operatorname{std}}(\boldsymbol{C}, \boldsymbol{Q}) + \hat{W}_{\operatorname{rem}}(\boldsymbol{C}, \boldsymbol{Q}, \operatorname{Grad}\boldsymbol{Q}), \quad (47a)$$

$$\hat{W}_{\text{rem}}(\boldsymbol{C}, \boldsymbol{Q}, \text{Grad}\boldsymbol{Q}) = \hat{W}_{\text{AC}}(\boldsymbol{C}, \boldsymbol{Q}) + \frac{1}{2}D_0 \|\text{Grad}\boldsymbol{Q}\|^2,$$
(47b)

$$\hat{W}_{\rm AC}(\boldsymbol{C}, Q) = \mathcal{A}_0 \hat{\mathcal{P}}(Q) \exp\left(\hat{\alpha}_W(\boldsymbol{C})Q\right), \tag{47c}$$

with $\hat{\alpha}_W(C)$ being defined in (46). Hence, we find

$$\begin{split} \hat{\boldsymbol{P}}_{\rm sc} &= \boldsymbol{F}\left(2\frac{\partial\hat{W}}{\partial\boldsymbol{C}}\right) = \boldsymbol{F}\left(2\frac{\partial\hat{W}_{\rm std}}{\partial\boldsymbol{C}}\right) + \boldsymbol{F}\left(2\frac{\partial\hat{W}_{\rm AC}}{\partial\boldsymbol{C}}\right) \\ &= \boldsymbol{F}\left(2\frac{\partial\hat{W}_{\rm std}}{\partial\boldsymbol{C}}\right) + \hat{W}_{\rm AC}Q\boldsymbol{F}\left(2\frac{\partial\hat{\alpha}_W}{\partial\boldsymbol{C}}\right) \end{split}$$

$$= \boldsymbol{F}\left(2\frac{\partial\hat{W}_{\text{std}}}{\partial\boldsymbol{C}}\right) + 2\hat{W}_{\text{AC}}(\boldsymbol{C},\boldsymbol{Q})\boldsymbol{Q}\,\boldsymbol{a}\left[I_{1}(\bar{\boldsymbol{C}}) - 3\right]J^{-2/3}\boldsymbol{F}\,\text{Dev}^{*}\boldsymbol{G}^{-1},\tag{48a}$$

$$\frac{\partial W}{\partial Q} = \frac{\partial W_{\text{std}}}{\partial Q} + \frac{\partial W_{\text{rem}}}{\partial Q} = \frac{\partial W_{\text{std}}}{\partial Q} + \frac{\partial W_{\text{AC}}}{\partial Q}$$

$$= \frac{\partial \hat{W}_{\text{std}}}{\partial Q} + \mathcal{A}_0 \frac{\partial \hat{\mathcal{P}}}{\partial Q} e^{\hat{\alpha}_W Q} + \mathcal{A}_0 \hat{\mathcal{P}} e^{\hat{\alpha}_W Q} \hat{\alpha}_W,$$
(48b)

where $\text{Dev}^* \boldsymbol{G}^{-1} := \boldsymbol{G}^{-1} - \frac{1}{3} (\boldsymbol{G}^{-1} : \boldsymbol{C}) \boldsymbol{C}^{-1}$ is the deviatoric part of \boldsymbol{G}^{-1} with respect to the deformed metric tensor \boldsymbol{C} . In particular, it holds that

$$\frac{\partial \hat{W}_{\text{std}}}{\partial Q} = \frac{\Phi_{1\text{s}}}{\omega^2} \text{cov} \left(\Theta, \hat{W}_{1\text{a}}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi))\right) \\
= \Phi_{1\text{s}} \frac{\langle\!\langle \Theta \hat{W}_{1\text{a}}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi)) \rangle\!\rangle - \langle\!\langle \Theta \rangle\!\rangle \langle\!\langle \hat{W}_{1\text{a}}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi)) \rangle\!\rangle}{\omega^2}, \quad (49\text{a})$$

$$\frac{\partial \hat{\mathcal{P}}}{\partial Q} = \frac{4}{(\pi/4)^4} Q \left(Q - \frac{\pi}{2} \right) \left(Q - \frac{\pi}{4} \right), \tag{49b}$$

where the notation $\mathbf{A} = \hat{\mathbf{A}}(\Theta, \Phi)$ means that the structure tensor has to be rewritten as a function of the angular coordinates Θ and Φ . The right-handside of (49a) is the covariance between Θ and $\hat{W}_{1a}(\mathbf{C}, \hat{\mathbf{A}}(\Theta, \Phi))$ and, since it involves the computation of directional averages, it has to be understood as a function of Q. In summary, the model equations are given by

Div
$$\left[-Jpg^{-1}F^{-T} + F\left(2\frac{\partial\hat{W}}{\partial C}\right)\right] = \mathbf{0},$$
 (50a)

$$\dot{J} = \operatorname{Div}\left(\boldsymbol{K}\operatorname{Grad}p\right),$$
(50b)

$$\Gamma \dot{Q} = -\left[\frac{\partial \hat{W}}{\partial Q} - \operatorname{Div}\left(D_0 \boldsymbol{G}^{-1} \operatorname{Grad} Q\right)\right] + \mathcal{R}_{\text{ext}}, \qquad (50c)$$

where the constitutive results reported in (48a)–(49b) have to be used. For the numerical computations we use the assumption that the model parameters depend only on the axial normalised coordinate $\xi = X^3/L \in [0, 1]$, with X^3 being the axial coordinate of the point $X \in \mathcal{B}$. In particular, the volumetric fractions Φ_{0s} , Φ_{1s} , and Φ_{s} are given by

$$\Phi_{0s} \equiv \Phi_{0s}(\xi) = -0.062\,\xi^2 + 0.038\,\xi + 0.046,\tag{51a}$$

$$\Phi_{1s} \equiv \Phi_{1s}(\xi) = +0.062\,\xi^2 - 0.138\,\xi + 0.204,\tag{51b}$$

$$\Phi_{\rm s} \equiv \Phi_{\rm s}(\xi) = -0.100\,\xi + 0.250. \tag{51c}$$

We also introduce the void ratio $e_{\rm R}(\xi) = (1 - \Phi_{\rm s}(\xi))/\Phi_{\rm s}(\xi)$, which is completely defined by (51c). Then, we prescribe the reference scalar permeability $k_{0\rm R}$ used $_{662}$ in (13) to be [59, 38]

$$k_{0\mathrm{R}} \equiv k_{0\mathrm{R}}(\xi) = k_{0\mathrm{R}}^{(0)} \left[\frac{e_{\mathrm{R}}(\xi)}{e_{\mathrm{R}}^{(0)}} \right]^{\kappa_0} \exp\left(\frac{1}{2}m_0 \left[\left(\frac{1+e_{\mathrm{R}}(\xi)}{1+e_{\mathrm{R}}^{(0)}}\right)^2 - 1 \right] \right), \quad (52)$$

with $k_{0R}^{(0)} = 0.003 \,\mathrm{mm^4 N^{-1} s^{-1}}$, $\kappa_0 = 0.0848$, $m_0 = 4.638$ [46], and $e_{R}^{(0)} = 4.0$ 663 [60]. For the "standard" part of the free energy density, $\hat{W}_{\rm std}$, we adopt the 664 parameters $\alpha_0 = 0.1250 \text{ MPa}$, $\alpha_1 = 0.7778$, $\alpha_2 = 0.1111$, and c = 7.5 MPa665 [61] for \hat{W}_0 , \hat{W}_{1i} , and \hat{W}_{1a} (see [38] and the reference therein), and q = 2, 666 r = 1/2, and $J_{\rm cr}(\xi) = \Phi_{\rm s}(\xi) + 0.1$ for the penalty term \hat{U} . For the remodelling 667 part, \hat{W}_{rem} , we use several pairs of D_0 and \mathcal{A}_0 (an example of such values is 668 $D_0 = 1.0 \cdot 10^{-4} \,\mathrm{N/rad}$ and $\mathcal{A}_0 = 154 \,\mathrm{Pa}$) and we let a take the values a = 0669 or $a = 10^3$ (clearly, also other values may be chosen). Finally, although in a 670 previous paper [54] we took the function 671

$$\omega(\xi) = 10^3 [(1 - \xi)\xi]^4 + 0.03 \tag{53}$$

to compute the variance $[\omega(\xi)]^2$, in the simulations performed for this work, we set $\omega(\xi) = \omega_0 = 0.3$ for all $\xi \in [0, 1]$.

⁶⁷⁴ 4 The remodelling equation

In this section, we study two limit cases of the remodelling equation. The first case shows that a stationary solution of the remodelling equation recovers the profile taken from [54], which mimics the histological pattern of fibre orientation. In the second case, we search for those stationary solutions to (50c) that may represent admissible target profiles of the remodelling variable. The existence of these solutions depends on the choice of the boundary conditions.

⁶⁸¹ 4.1 The histological profile

As anticipated in Section 3.2, the reason for choosing the functional forms (21)– (27) is histological. To see this, let us assume that the reference, undeformed configuration of the sample coincides with the region of space that it occupies at time t = 0. In this configuration, the pattern of the fibre orientation can be observed experimentally, and an expression of the mean angle fitting the histological data is given by [54]

$$Q_{\rm fit}(\xi) = \frac{\pi}{2} \left\{ 1 - \cos\left(\frac{\pi}{2} \left[-\frac{2}{3}\xi^2 + \frac{5}{3}\xi \right] \right) \right\},\tag{54}$$

where ξ is the normalised axial coordinate. The coordinate ξ is zero at the bone-cartilage interface (also known as "tidemark"), which coincides with the sample's lower boundary $(\partial \mathcal{B})_{L}$, and is equal to unity at the articular surface, represented by the upper boundary $(\partial \mathcal{B})_{U}$. Note that, in this configuration, the fluid is assumed to be at rest and the pore pressure is taken equal to zero everywhere in the tissue. The function $Q_{\rm fit}$ takes the values $Q_{\rm fit}(0) = 0$ rad and $Q_{\rm fit}(1) = \pi/2$ rad, thereby meaning that the fibres are almost perfectly parallel to the specimen's symmetry axis at the tidemark, and almost perfectly orthogonal to it at the articular surface. Thus, by construction, $Q_{\rm fit}$ mimics the histological profile of the fibre mean angle.



Fig. 2 (a): Comparison between $Q_{\text{fit}}(\xi)$ and $Q(\xi)$ for a given set of parameters \mathcal{A}_0 , D_0 , and specimen height L. For the chosen parameters, the two curves deviate appreciably from each other only for values of ξ close to zero, i.e., in the deep zone of articular cartilage. (b): The Allen-Cahn free energy density in (26) is represented. The dashed parts lie outside of the considered range $[0, \pi/2]$. In fact, the two minima correspond to Q(0) = 0 rad and $Q(1) = \pi/2$ rad, respectively.

We take inspiration from the aforementioned experimental observations 698 to claim that the angles $Q_{\rm fit}(0) = 0$ rad and $Q_{\rm fit}(1) = \pi/2$ rad are "critical" 699 values of the fibre mean angle and, more importantly, that the histological 700 profile is the result of a "structural phase transition" occurring in articular 701 cartilage at some stage of its formation (thus, *prior* to any mechanical test 702 performed on the tissue either in vitro or in silico). In our view, this phase 703 transition consists of a structural reorganisation of the tissue, and leads to 704 the histological fibre distribution observed in the undeformed configuration. 705 To see whether our interpretation is compatible with experimental evidence, 706 we endow the tissue with a free energy density of the Allen-Cahn type, which 707 we assume to exist independently of deformation, and we suggest that the 708 histological profile is the solution of a variational problem formulated in the 709 undeformed configuration. In fact, we choose $\hat{W}_{\text{rem}}^{(0)}(Q, \text{Grad } Q)$ as specified in (24a), with $\hat{W}_{\text{str}}^{(0)}(Q) = \hat{W}_{\text{AC}}^{(0)}(Q)$ as in (26), and we require the functional derivative of $\mathcal{W}_{\text{rem}}^{(0)}$ [see Eq. (25)] to be zero. This amounts to solving the partial 710 711 712 differential equation 713

$$\frac{\partial \hat{W}_{\rm rem}^{(0)}}{\partial Q} - \text{Div}\left[\frac{\partial \hat{W}_{\rm rem}^{(0)}}{\partial \text{Grad}\,Q}\right] = 0 \quad \Rightarrow \tag{55a}$$

$$\frac{\partial \hat{W}_{\rm AC}^{(0)}}{\partial Q} - \operatorname{Div}\left[D_0 \boldsymbol{G}^{-1} \operatorname{Grad} Q\right] = 0 \quad \Rightarrow \tag{55b}$$

$$\frac{4\mathcal{A}_0}{(\pi/4)^4}Q\left(Q-\frac{\pi}{2}\right)\left(Q-\frac{\pi}{4}\right) - \operatorname{Div}\left[D_0\boldsymbol{G}^{-1}\operatorname{Grad}Q\right] = 0.$$
(55c)

Let us now focus on a particularly simple case in which the sample is a cylinder (as specified in section 3.4), and Q depends only on the normalised axial coordinate ξ . The coefficient D_0 is set equal to zero from the outset when the spatial resolution of the remodelling variable is not explicitly taken into account, and is greater than zero otherwise. According to these hypotheses, when $D_0 \neq 0$, (55c) becomes

$$\frac{4\mathcal{A}_0 L^2}{(\pi/4)^4 D_0} Q\left(Q - \frac{\pi}{2}\right) \left(Q - \frac{\pi}{4}\right) - \frac{\mathrm{d}^2 Q}{\mathrm{d}\xi^2} = 0,\tag{56}$$

with the boundary conditions Q(0) = 0 rad and $Q(1) = \pi/2$ rad. Comparing 720 the solution of (56), $Q_{\rm h}(\xi)$, with the function $Q_{\rm fit}(\xi)$ assigned in (54) allows 721 to estimate the combination of parameters \mathcal{A}_0 and D_0 that minimises the 722 distance between $Q_{\rm h}(\xi)$ and $Q_{\rm fit}(\xi)$ (see Fig. 2). This result seems to suggest 723 that, after the model parameters are calibrated on the basis of experimental 724 observations, and the histologically based boundary conditions Q(0) = 0 rad 725 and Q(1) = 0 rad are enforced, the functional form of the histological profile 726 need not be prescribed by fitting experimental data, since it may be computed 727 as the extremum of the remodelling energy (25). 728

As anticipated in Section 3.4, the Dirichlet boundary conditions imposed 729 on the values taken by Q at the lower and upper boundary of the sample 730 enhance the convergence of the solution towards $Q_{\rm fit}$. This behaviour, however, 731 manifests itself only at $(\partial \mathcal{B})_{L}$ and $(\partial \mathcal{B})_{U}$, where the conditions (45a) and 732 (45b) comply with the minimum configurations of $\hat{W}^{(0)}_{AC}(Q)$. In general, instead, 733 when the evolution of the fibre mean angle is studied in conjunction with the 734 deformation of the tissue, our model can produce a profile that is far from 735 the histological one (see e.g. Fig. (8)). Moreover, other boundary conditions, 736 which may depend on time, deformation, or stress, could also be considered 737 to better describe other physical occurrences. 738

⁷³⁹ We remark that the profile reported in Fig. 2(a) has been obtained for ⁷⁴⁰ L = 1 mm and the ratio $(\mathcal{A}_0 L^2)/D_0 = 1.54$. A pair of model parameters ⁷⁴¹ \mathcal{A}_0 and D_0 complying with this ratio is given by $D_0 = 1.0 \cdot 10^{-4} \text{ N/rad}$ and ⁷⁴² $\mathcal{A}_0 = 154 \text{ Pa}$.

743 4.2 "Target fields" and stationary solutions

An essential issue in the mechanical theories of remodelling is the identification of the generalised forces that drive the structural evolution of the considered system. Before studying this problem within our theoretical framework, we review the case in which the free energy density does not feature terms of the type $\hat{W}_{\rm rem}(\boldsymbol{C}, \boldsymbol{Q}, {\rm Grad} \boldsymbol{Q})$. In such a setting, the remodelling law (50c) reduces to the ordinary differential equation

$$\Gamma \dot{Q} = \Re_{\text{ext}} - \frac{\partial \dot{W}_{\text{std}}}{\partial Q} (\boldsymbol{C}, Q), \qquad (57)$$

⁷⁵⁰ and the evolution of Q is entirely driven by the difference between \mathcal{R}_{ext} and ⁷⁵¹ $\partial \hat{W}_{std}/\partial Q$. More specifically, while $\partial \hat{W}_{std}/\partial Q$ is dictated by the choice of \hat{W}_{std} , ⁷⁵² \mathcal{R}_{ext} characterises the coupling between Q and the other mechanical variables ⁷⁵³ of the system. For example, following Hariton et al. [62], \mathcal{R}_{ext} may be related ⁷⁵⁴ to stress by claiming that the direction along which the fibres tend to align

themselves is driven by the eigenvalues of Cauchy stress tensor. To account

⁷⁵⁶ for this requirement, it is possible to prescribe
$$\mathcal{R}_{ext}$$
 as [27]

$$\mathcal{R}_{\text{ext}} \equiv \frac{\partial W_{\text{std}}}{\partial Q} (\boldsymbol{C}, Q_{\text{T}}), \tag{58}$$

where $Q_{\rm T}$ is a suitably constructed *target angle*, i.e., a "privileged" distribution of the mean angle entirely determined by stress. We emphasise that, since the principal stresses are time-dependent, the target angle varies in time [27]. Thus, \dot{Q} is generally non-zero until Q is not equal to $Q_{\rm T}$. If, however, (57) and (58) are studied in the limit in which $Q_{\rm T}$ tends to some stationary distribution $Q_{\rm T}^{\infty}$, the remodelling process ceases asymptotically when Q approaches one of the stationary solutions of the evolution equation

$$\Gamma \dot{Q} = \frac{\partial \dot{W}_{\text{std}}}{\partial Q} (\boldsymbol{C}, Q_{\text{T}}^{\infty}) - \frac{\partial \dot{W}_{\text{std}}}{\partial Q} (\boldsymbol{C}, Q).$$
(59)

⁷⁶⁴ In particular, if the dependence of \hat{W}_{std} on Q implies the uniqueness of the ⁷⁶⁵ stationary solution to (59), then $Q_{st} \equiv Q_T^{\infty}$ is the stationary mean angle ⁷⁶⁶ towards which the system remodels.

We remark that the existence of solutions of the type $Q_{\rm st} = Q_{\rm T}^{\infty}$ is closely related to the introduction of the target angle and the external remodelling force, $\mathcal{R}_{\rm ext}$. In a previous work [39], however, we searched for stationary solutions to (57) in the limit case of vanishing, or negligibly small, $\mathcal{R}_{\rm ext}$ and with $\hat{W}_{\rm std}$ defined as in (18)–(20c). Consequently, we solved the remodelling equation

$$\Gamma \dot{Q} = -\frac{\partial \hat{W}_{\text{std}}}{\partial Q},\tag{60}$$

and we found that \dot{Q} tended asymptotically towards zero because the condition

$$0 = -\frac{\partial \hat{W}_{\text{std}}}{\partial Q} = -\frac{\Phi_{1\text{s}}}{\omega^2} \text{cov}\left(\Theta, \hat{W}_{1\text{a}}(\boldsymbol{C}, \boldsymbol{\hat{A}}(\Theta, \Phi))\right)$$
(61)

applied for large values of t. This result was respected because the deformation obtained for large values of t implied the asymptotic fulfilment of the inequality $I_4 \leq 1$, even though (61) admitted no roots in the variable Q. We remark a *posteriori* that, if \mathcal{R}_{ext} had been considered in [39] in the form given in (58), the presence of the Heaviside function $\mathcal{H}(I_4-1)$ in the definition of \hat{W}_{std} would have made it tend asymptotically towards zero for the deformations attained in the tissue for large times.

The theoretical setting developed in this work is conceived to improve 781 the results obtained in [39]. To this end, it proposes to describe remodelling 782 through (50c), which introduces two novelties: It accounts for the spatial res-783 olution of the fibre mean angle, and it defines the remodelling part of the sys-784 tem's free energy density, \hat{W}_{rem} , where $\exp(\hat{\alpha}_W(C)Q)$ describes a non-trivial 785 coupling between Q and the deformation [see (31b) and (28)]. By enforcing 786 the simplifying assumptions done in Section 3.4, and neglecting \mathcal{R}_{ext} from the 787 outset, the remodelling equation (50c) becomes 788

$$\Gamma \dot{Q} = \operatorname{Div} \left[D_0 \boldsymbol{G}^{-1} \operatorname{Grad} Q \right] - \frac{\partial W_{\mathrm{AC}}}{\partial Q} - \frac{\partial W_{\mathrm{std}}}{\partial Q}.$$
(62)

⁷⁸⁹ Note that, similarly to \mathcal{R}_{ext} in (57), also the term $-\partial \hat{W}_{AC}/\partial Q$ plays a "driving" ⁷⁹⁰ role in the evolution of the fibre mean angle and, in fact, we switch off \mathcal{R}_{ext} with ⁷⁹¹ the purpose of focussing on the implications of $-\partial \hat{W}_{AC}/\partial Q$ on remodelling. ⁷⁹² In this case, since no stress-driven target angle is considered *a priori* in the ⁷⁹³ model, $-\partial \hat{W}_{AC}/\partial Q$ modulates the evolution of Q through the deformation. ⁷⁹⁴ In this framework, however, a "target angle" is —if it exists— a stationary ⁷⁹⁵ solution to (62), i.e., a function obtained by solving

$$-\left[\frac{\partial \hat{W}_{\rm std}}{\partial Q} + \frac{\partial \hat{W}_{\rm AC}}{\partial Q} - \operatorname{Div}\left(D_0 \boldsymbol{G}^{-1} \operatorname{Grad} Q\right)\right] = 0, \tag{63}$$

together with (50a), (50b), and the boundary conditions prescribed in Section 796 3.4. For example, in the case of articular cartilage, we impose Q(X) = 0 rad 797 for $X \in (\partial \mathcal{B})_{\mathrm{L}}$ and $Q(X) = \pi/2$ rad for $X \in (\partial \mathcal{B})_{\mathrm{U}}$, thereby requiring the 798 congruence of Q with the initial histological data for all the points of the 799 lower boundary, $(\partial \mathcal{B})_{L}$, and for all the points of the upper boundary, $(\partial \mathcal{B})_{U}$, 800 of the cartilage specimen taken for benchmarking (note that the dependence 801 of Q on time has been suppressed here, because we are looking for stationary 802 solutions). We notice that, notwithstanding their similar form, (63) is quite 803 different from (55c). The differences are essentially due to two facts. Firstly, in 804 (63), both the contribution to remodelling stemming from the standard strain 805 energy density, $\dot{W}_{\rm std}$, and the Allen-Cahn contribution, $\dot{W}_{\rm AC}$, are accounted 806 for. Secondly, in (63), W_{AC} takes into account the coupling between deforma-807 tion and remodelling, since it depends both on C and on Q. In particular, the 808 introduction of the factor $\exp(\hat{\alpha}_W(C)Q)$ shifts, for a given C, the maximum 809 configuration of $\hat{W}_{AC}(\boldsymbol{C}, \boldsymbol{Q})$ from $\pi/4$ to the deformation dependent value 810

$$Q_{\max} \equiv Q_{\max}(\mathbf{C}) = \frac{-8 + \pi \hat{\alpha}_W(\mathbf{C}) + \sqrt{64 + \pi^2 [\hat{\alpha}_W(\mathbf{C})]^2}}{4 \hat{\alpha}_W(\mathbf{C})}, \qquad (64)$$

for $\hat{\alpha}_W(\mathbf{C}) \neq 0$. In the limit of vanishing $\hat{\alpha}_W(\mathbf{C})$, the value $Q_{\text{max}} = \pi/4$ rad is recovered.

In the following, we speak of "standard remodelling" when we refer to (60),

and we call "non-standard remodelling" the process described by (62).

815 5 Numerical Tests

In this section, we report the results of the Finite Element implementation of the unconfined compression test described in Section 3.4. To this end, we consider the weak form of the model equations (50a)-(50c) associated with the BCs (43a)-(43c) and (45a)-(45c), i.e.,

$$\mathcal{F}(\chi, p, Q) = \mathcal{F}_{\chi}(\chi, p, Q) + \mathcal{F}_{p}(\chi, p, Q) + \mathcal{F}_{Q}(\chi, Q) = 0,$$
(65)

where the functionals \mathcal{F}_{χ} , \mathcal{F}_{p} , and \mathcal{F}_{Q} are defined as

$$\mathcal{F}_{\chi}(\chi, p, Q) = \int_{\mathcal{B}} \left[-Jp \, \boldsymbol{g}^{-1} \boldsymbol{F}^{-\mathrm{T}} + \hat{\boldsymbol{P}}_{\mathrm{sc}}(\boldsymbol{F}, Q) \right] : \boldsymbol{g} \operatorname{Grad} \boldsymbol{\tilde{u}}, \tag{66a}$$

$$\mathcal{F}_{p}(\chi, p, Q) = \int_{\mathcal{B}} \left[\dot{J}\tilde{p} + (\operatorname{Grad}\tilde{p})\hat{K}(\boldsymbol{C}, Q)(\operatorname{Grad}p) \right],$$
(66b)

$$\begin{aligned} \mathcal{F}_{Q}(\chi,Q) &= \int_{\mathcal{B}} \left[D_{0} \boldsymbol{G}^{-1} \operatorname{Grad} Q \right] \operatorname{Grad} \tilde{\Omega} \\ &+ \int_{\mathcal{B}} \left[\Gamma \dot{Q} + \frac{\partial \hat{W}_{\mathrm{std}}}{\partial Q} (\boldsymbol{C},Q) + \frac{\partial \hat{W}_{\mathrm{AC}}}{\partial Q} (\boldsymbol{C},Q) \right] \tilde{\Omega}. \end{aligned} \tag{66c}$$

Here, $\tilde{\boldsymbol{u}}$ and $\tilde{\Omega}$ are the test velocities associated with the solid phase motion, χ , and the mean angle, Q, respectively, and \tilde{p} is the test pressure.

Equations (66a)–(66c) are discretised in time and, at each time step, they 823 are solved with the aid of a linearisation method. This requires to compute 824 the directional averages that define \hat{P}_{sc} , \hat{K} , and $\partial \hat{W}_{std}/\partial Q$, along with their 825 derivatives (such derivatives, indeed, appear in the linearisation scheme). In 826 fact, the evaluation of these averages is accomplished by having recourse to the 827 numerical procedure known as Spherical Design Algorithm (SDA) [63]. Since 828 presenting the whole procedure is rather lengthy and out of the scope of our 829 work, we show here only the construction of $\partial \hat{W}_{std} / \partial Q$ (see algorithm A1). 830

⁸³¹ 5.1 Remodelling in the absence of deformation

In this section, we solve (62) independently of deformation. Such a situation 832 occurs when no load is applied to the tissue (i.e., g(t) is zero for all times), 833 the pore pressure is null at all times and at all points of the tissue, and no 834 external force (such as the gravitational force) is considered. Hence, the sample 835 is assumed to lean on the support beneath and its lower surface can be assumed 836 to be free of surface forces. In this case, the balance laws (50a) and (50b) are 837 trivially satisfied, and the term $\partial \hat{W}_{\rm std} / \partial Q$ vanishes identically, so that the 838 remodelling equation (62) becomes 839

$$\Gamma \dot{Q} = \operatorname{Div} \left[D_0 \boldsymbol{G}^{-1} \operatorname{Grad} \boldsymbol{Q} \right] - \frac{\partial \dot{W}_{\mathrm{AC}}}{\partial \boldsymbol{Q}}, \tag{67}$$

840 with

$$\frac{\partial \hat{W}_{\rm AC}}{\partial Q}(\boldsymbol{G}, Q) = \mathcal{A}_0 \frac{\partial \hat{\mathcal{P}}}{\partial Q}(Q) = \frac{4\mathcal{A}_0}{(\pi/4)^4} Q\left(Q - \frac{\pi}{2}\right) \left(Q - \frac{\pi}{4}\right).$$
(68)

We solve now (67) with the BCs (45a)–(45c) and under the hypothesis that, at the initial time of observation, the fibre mean angle Q(X,0) is a random function of X. Hence, the tissue finds itself in a disordered configuration at the initial time. We make this assumption in order to show that the Allen-Cahn model, along with the BCs (45a)–(45c), is capable of describing a change of the tissue's material symmetry, which converts from the disordered configuration towards the ordered configuration that renders it transversely isotropic.



Fig. 3 Stationary profiles of the remodelling variable for different values of D_0 , with $A_0 = 247$ Pa (a), and for different values of A_0 , with $D_0 = 1.0 \cdot 10^{-4}$ N/rad (b). The grey circled curve in the plot on the left represents the initial profile of Q, which is set to be random.

The results of the initial-boundary value problem specified by (67), (68), 848 and (45a)-(45c) are shown in Fig. 3 for varying values of the parameters D_0 (cf. 849 Fig. 3a) and \mathcal{A}_0 (cf. Fig. 3b). Starting from a random profile (grey circled curve 850 in Fig. 3a), which might represent the orientation of the fibres in an engineered 851 tissue [64], Q(X,t) evolves towards a stationary solution that is remnant of 852 the histological profile reported in Fig. 2a. This behaviour is a consequence of 853 the introduction of the Allen-Cahn energy density, W_{AC} , whose two minimum 854 configurations coincide with the boundary values imposed on Q, and manifests 855 itself through the tendency of the remodelling variable to acquire a stationary 856 solution interpolating between the imposed Dirichlet boundary conditions at 857 the top (cf. (45a)) and at the bottom (cf. (45b)) of the sample. We remark that 858 the free energy \hat{W}_{AC} generates a profile that is comparable with the histological 859 one. In this respect we say that, in principle, the remodelling may occur also 860 in the absence of deformation, and may be understood as a structural phase 861 transition. Indeed, the system passes from a "phase" in which it appears to 862 be disordered to a "phase" in which it is ordered in such a way that it is 863 transversely isotropic. This loss, or *breaking*, of the system's symmetries is due 864 to the introduction of W_{rem} . 865

⁸⁶⁶ 5.2 Asymptotic "standard remodelling"

We launch a first set of simulations in which $\Re_{ext} = 0$ and the free energy 867 density is equal to the standard one only, i.e., $W = W_{std}$. In this case, the 868 remodelling equation is given by (60) rather than (50c) and, as anticipated 869 in Section (4.2), Q tends towards zero for large values of t because (61) is re-870 spected asymptotically. To see why this occurs, it is necessary to determine I_4 871 and construct the derivative $\partial \hat{W}_{\rm std} / \partial Q$. The latter, in turn, requires to evalu-872 ate the directional averages reported in (49a) and, thus, to use the Spherical 873 Design Algorithm [63]. Indeed, for a given C, $\partial \hat{W}_{std}/\partial Q$, is approximated as 874

$$\frac{\partial \hat{W}_{\text{std}}}{\partial Q}(\boldsymbol{C},Q) = \frac{\Phi_{1s}}{\omega^2} \operatorname{cov}\left(\Theta, \hat{W}_{1a}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi))\right) \\
= \frac{\Phi_{1s}}{\omega^2} \langle\!\!\langle (\Theta - \langle\!\!\langle \Theta \rangle\!\!\rangle) \, \hat{W}_{1a}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi)) \rangle\!\!\rangle \\
= \frac{\Phi_{1s}}{\omega^2} \int_0^{2\pi} \!\!\!\int_0^{\pi/2} \left(\Theta - \langle\!\!\langle \Theta \rangle\!\!\rangle\right) \, \hat{W}_{1a}(\boldsymbol{C}, \hat{\boldsymbol{A}}(\Theta, \Phi)) \hat{\wp}(\Theta) \sin(\Theta) \mathrm{d}\Theta \mathrm{d}\Phi \\
\approx \frac{\Phi_{1s}}{\omega^2} \frac{2\pi}{N} \sum_{i=1}^m \sum_{j=1}^n \left(\Theta_i - \langle\!\!\langle \Theta \rangle\!\!\rangle\right) \, \hat{W}_{1a}(\boldsymbol{C}, \boldsymbol{A}_{ij}) \hat{\wp}(\Theta_i),$$
(69)

where N = mn is the total number of quadrature points used for the numerical solution of the integral in (69), $\Im \times \Im \subset [0, \pi/2] \times [0, \pi]$ is the set of all quadrature points, and, for each $(\Theta_i, \Phi_j) \in \Im \times \Im$, we write $A_{ij} = M_{ij} \otimes M_{ij}$ (no sum with respect to *i* and *j*), with $M_{ij} = \hat{M}(\Theta_i, \Phi_j)$. Hence, $\hat{W}_{1a}(C, A_{ij})$ is rewritten as

$$\hat{W}_{1a}(\boldsymbol{C}, \boldsymbol{A}_{ij}) = \mathcal{H}\left(I_4(\boldsymbol{C}, \boldsymbol{A}_{ij}) - 1\right) \frac{1}{2} c \left[I_4(\boldsymbol{C}, \boldsymbol{A}_{ij}) - 1\right]^2.$$
(70)

Note that \mathcal{J} and \mathcal{J} are sets of points suitably chosen in $[0, \pi/2]$ and $[0, 2\pi]$, respectively [40].

As prescribed in lines 21 and 22 of the pseudo-code of Algorithm A1, the summand of (69) with indices *i* and *j* contributes to $\partial \hat{W}_{std}/\partial Q$ only if $\hat{\wp}(\Theta_i)$ is greater than a given threshold value, tol_{Ψ} , and $I_4(C, A_{ij}) > 1$. The first control is, in fact, on the probability density that a fibre is aligned along the direction specified by $(\Theta_i, \Phi_j) \in J \times \mathcal{J}$. The second condition, instead, represents the algorithmic formulation of the Heaviside function in (70).

To have indications about these restrictions, we study the time evolution 888 of $I_4(C, A_{ij})$ and $\hat{\wp}$ at two selected points of the sample, for different values 889 of Θ . The results are reported in Fig. 4, where the black curves represent 890 constant values for I_4 and $\hat{\wp}$, taken as reference (here, we choose $I_4^{(0)} = 1$ 891 and $\hat{\wp}^{(0)} = \operatorname{tol}_{\Psi}$). Moreover, the point of coordinates $X_{\rm L} = (0, 0, L/4)$ finds 892 itself in the deep zone of the sample, in which the fibres tend to be parallel 893 to the symmetry axis of the cylinder and, thus, perpendicular to the lower 894 boundary (this corresponds to the bone-cartilage interface when the tissue is 895 in vivo). The point of coordinates $X_{\rm U} = (0, 0, 3L/4)$, instead, is situated in 896

(100) and (00) while the per time step and the ten internet sector internet
1: procedure SDA
2: for $k = 1,, M$ do (M is the number of grid nodes)
3: Initialise $\left(\frac{\partial \hat{W}_{\text{std}}}{\partial Q}\right)^{p\ell k} = 0$, and $\mathcal{Z}^{p\ell k} = 2\pi \int_0^{\pi/2} \hat{\gamma}^{p\ell k}(\Theta) \sin \Theta d\Theta = 0$ (partial sums)
4: Load the point set $\{(\Theta_i, \Phi_j)\}_{i,j=1}^{N=mn} \subset \mathcal{I} \times \mathcal{J}$
5: Load $Q^{p\ell k} = Q^{\ell}(X_k, t_p)$ and $\omega^k = \omega(\xi_k)$
6: for $i = 1,, m$ do (inner cycle to evaluate the normalisation factor)
7: Evaluate $\hat{\gamma}^{p\ell k}(\Theta_i) = \exp\left(-\frac{\left(\Theta_i - Q^{p\ell k}\right)^2}{2\left[\omega^k\right]^2}\right)$
8: $\mathcal{Z}^{p\ell k} = \mathcal{Z}^{p\ell k} + \frac{2\pi}{N} \hat{\gamma}^{p\ell k}(\Theta_i)$
9: end for
10: Calculate $\hat{\wp}^{p\ell k}(\Theta_i) = \frac{\hat{\gamma}^{p\ell k}(\Theta_i)}{z^{p\ell k}}, \ i = 1, \dots, m$
11: for $i = 1,, m$ do inner cycle to determine $\langle \Theta \rangle^{p\ell k}$
12: if $\hat{\wp}^{p\ell k}(\Theta_i) > \operatorname{tol}_{\Psi}$ then
13: $\langle \Theta \rangle^{p\ell k} = \langle \Theta \rangle^{p\ell k} + \frac{2\pi}{N} \Theta_i \hat{\wp}^{p\ell k} (\Theta_i)$
14: end if
15: end for
16: Given $C^{p \iota \kappa}$:
$1'$: for $i = 1, \dots, m$ do
18: for $j = 1, \dots, n$ do
19: Evaluate $I_4(C^{pere}, A_{ij}) = C^{pere} : A_{ij}$, and
20: $A_{ij} = M_{ij} \otimes M_{ij}$, with $M_{ij} = M(\Theta_i, \Phi_j)$
21: if $\hat{\varphi}^{p\ell k}(\Theta_i) > \operatorname{tol}_{\Psi}$ then
22: if $I_4(\boldsymbol{C}^{p\ell k}, \boldsymbol{A}_{ij}) > 1$ then
23: Evaluate
24: $\mathcal{R}^{p\ell k}(\Theta_i, \Phi_j) = \frac{\Phi_{1s}(X_k)}{[\omega^k]^2} \left(\Theta_i - \langle \Theta \rangle\right) \frac{1}{2} c \left[I_4(\boldsymbol{C}^{p\ell k}, \boldsymbol{A}_{ij}) - 1 \right]^2 \hat{\wp}^{p\ell k}(\Theta_i)$
25: $\left(\frac{\partial \hat{W}_{\text{std}}}{\partial Q}\right)^{p\ell k} = \left(\frac{\partial \hat{W}_{\text{std}}}{\partial Q}\right)^{p\ell k} + \frac{2\pi}{N} \mathcal{R}^{p\ell k}(\Theta_i, \Phi_j)$
26: end if
27: end if
28: end for
29: end for
30: end for
31: end procedure

Algorithm 1 -A5- Spherical Design Algorithm (SDA) for the evaluation of (49a) and (69) within the *p*th time step and the ℓ th linearisation iteration

the superficial zone, in which the fibres are parallel to the upper boundary (which corresponds to the articular surface of the tissue *in vivo*).

Looking at the left column of Fig. 4, obtained for $X_{\rm U} = (0, 0, 3L/4)$, we see 899 that the curves corresponding to $I_4(C, \hat{A}(2\pi/5, \Phi))$ and $I_4(C, \hat{A}(\pi/2, \Phi))$ are 900 above 1 for all the duration of the experiment, and tend to unity from above 901 for large times. Thus, at least in principle, the fibres aligned along $M(2\pi/5, \Phi)$ 902 and $\hat{M}(\pi/2, \Phi)$ contribute to $\partial \hat{W}_{std}/\partial Q$. However, the corresponding probabil-903 ity densities become smaller than tol_{\varPsi} as times goes by, thereby ruling out the 904 fibres oriented parallel to $\hat{M}(2\pi/5, \Phi)$ and $\hat{M}(\pi/2, \Phi)$. The curve correspond-905 ing to $I_4(\mathbf{C}, \hat{\mathbf{A}}(\pi/3, \Phi))$ is above 1 up to a certain instant of time subsequent 906 $T_{\rm ramp}$, and goes below 1 afterwards. Thus, the fibres aligned along $\hat{M}(\pi/3, \Phi)$ 907 do not contribute to $\partial \hat{W}_{\rm std}/\partial Q$. Finally, all other curves are below 1 for all 908 the duration of the experiment and give, then, no contribution to (69). 909

The right column of Fig. 4, which refers to $X_{\rm L} = (0, 0, L/4)$, shows that the curve $I_4(C, \hat{A}(\pi/2, \Phi))$ is the only one that remains above 1, even though it tends to unity for large values of t. The corresponding probability density, ⁹¹³ however, goes below $\operatorname{tol}_{\Psi}$ after T_{ramp} , thereby nullifying the contribution to ⁹¹⁴ (69) stemming from the fibres oriented along $\hat{M}(\pi/2, \Phi)$. In conclusion, Fig. 4 ⁹¹⁵ indicates that, for sufficiently large values of t, $\partial \hat{W}_{\mathrm{std}}/\partial Q$ tends towards zero ⁹¹⁶ because the deformation established in the sample and the values taken by the

⁹¹⁷ probability density switch off all the contributions of the sum (69).



Fig. 4 Time evolution of $I_4(C, \hat{A}(\Theta, \Phi))$ and $\bar{\wp}_X(\Theta)$ at $\Theta \in \mathbb{J} = \{0, \frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \frac{2\pi}{5}, \frac{\pi}{2}\}$. Note that, for the computed deformation, $I_4(C, \hat{A}(\Theta, \Phi))$ is independent of Φ . The figures in the left column correspond to the point of coordinates $X_U = (0, 0, 3L/4)$; those in the right column to the point of coordinates $X_L = (0, 0, L/4)$.

918 5.3 "Standard" versus "non-standard" remodelling

It is worth to remark that, as long as it holds that $\hat{W} = \hat{W}_{\text{std}}$, the parameter Γ 919 determines the stationary value of Q for a given loading time. Once this value 920 is reached, if no additional compression is applied to the sample, then Q = 0921 applies and no further evolution is observed. On the contrary, when the free 922 energy density is given by $\hat{W} = \hat{W}_{std} + \hat{W}_{rem}$, with \hat{W}_{rem} specified in (31b), 923 remodelling continues even when $\partial \hat{W}_{\rm std} / \partial Q$ becomes negligibly small. This 924 further evolution of the mean angle is induced by $W_{\rm rem}$ only. The described 925 behaviour is represented in Figs. 5 and 6, where the evolution of Q and $-\Gamma \dot{Q}$ 926 over time is shown both in the case of "standard" and in the case of "non-927 standard" remodelling. Note that Figs. 5 and 6 are obtained by evaluating Q928 in $X_{\rm L} = (0, 0, L/4)$ and $X_{\rm U} = (0, 0, 3L/4)$, respectively. 929

"Standard" remodelling predicts that both $Q(X_{\rm L}, t)$ and $Q(X_{\rm U}, t)$ decrease monotonically towards asymptotically constant values (see Figs. 5a and 6a). This behaviour is consistent with the trend of $-\Gamma \dot{Q}$ shown in Figs. 5b and 6b. Indeed, since $-\Gamma \dot{Q}(X_{\rm L}, t)$ and $-\Gamma \dot{Q}(X_{\rm U}, t)$ are both non-negative for all times, and Γ is strictly positive, the derivatives $\dot{Q}(X_{\rm L}, t)$ and $\dot{Q}(X_{\rm U}, t)$ are non-positive for all times. "Non-standard" remodelling, instead, destroys the



Fig. 5 (a): Time evolution of the mean angle Q. (b) Time evolution of $-\Gamma \dot{Q}$ (note that, in the label, the notation $Q_t \equiv \dot{Q}$ has been used). The dashed curves with asterisks refer to "standard" remodelling. The solid curves refer to "non-standard" remodelling for a = 0. All curves are obtained by evaluating both Q and $-\Gamma \dot{Q}$ in $X_{\rm L} = (0, 0, L/4)$. The units of Γ are J s m⁻³.



Fig. 6 (a): Time evolution of the mean angle Q. (b) Time evolution of $-\Gamma \dot{Q}$ (note that, in the label, the notation $Q_t \equiv \dot{Q}$ has been used). The dashed curves with asterisks refer to "standard" remodelling. The solid curves refer to "non-standard" remodelling for a = 0. All curves are obtained by evaluating both Q and $-\Gamma \dot{Q}$ in $X_{\rm U} = (0, 0, 3L/4)$. The units of Γ are J s m⁻³.

monotonicity of the curves $Q(X_{\rm L}, t)$ and $Q(X_{\rm U}, t)$, and slows down the rate by which they approach a stationary value.

From Fig. 5 we see that, in the case of "standard" remodelling, the variation 938 of both $Q(X_{\rm L},t)$ and $-\Gamma \dot{Q}(X_{\rm L},t)$ is markedly smaller than it is in the case 939 of "non-standard" remodelling. This behaviour is mainly due to the fact that 940 the initial preferential direction of the fibres is close to the one that is parallel 941 to the symmetry axis of the sample. Thus, for almost all fibres it holds $I_4 \leq 1$. 942 In other words, the term $-\Gamma \dot{Q}$ in (60) ("standard" case) is much smaller than 943 $-\Gamma \dot{Q}$ in (62) ("non-standard" case). In addition, we remark that, when the 944 free energy density \hat{W}_{rem} is introduced, the quantity $-\Gamma \dot{Q}(X_{\text{L}},t)$ is different 945 from zero at t = 0 s. This is due to the fact that, at t = 0 s, \hat{W}_{std} is equal to 946 the unessential constant α_0 , while \hat{W}_{rem} is non-trivial, because the gradient of 947 Q is not null at $X = X_{\rm L}$, and the value $Q(X_{\rm L}, 0) \approx 0.265 \,\mathrm{rad}$ is sufficiently 948 far away from the zeroes of $\partial \hat{W}_{AC}/\partial Q$ (at t = 0 s, they are Q = 0 rad, Q =949 $\pi/4$ rad, and $Q = \pi/2$ rad). For $t \ge 0, -\Gamma \dot{Q}(X_{\rm L}, t)$ grows during the first 950 instants of time of the loading ramp, thereby leading to a decrease of Q, 951

and reaches an absolute maximum. Then, it goes below zero and tends again towards an asymptotic value. This trend, however, seems not to be followed for $\Gamma = 5.0 \cdot 10^5 \,\mathrm{J\,s\,m^{-3}}$ (see Fig. 5b), even though both $Q(X_{\mathrm{L}}, t)$ and $-\Gamma \dot{Q}(X_{\mathrm{L}}, t)$ converge to stationary values for sufficiently long times.

In contrast to what is observed in Fig. 5, we see in Fig. 6 that \hat{W}_{rem} does 956 not affect appreciably the trend of the remodelling variable in the course of 957 the loading ramp, i.e., for $t \in [0, T_{\text{ramp}}]$. For $t \ge T_{\text{ramp}}$, instead, the "standard" 958 remodelling predicts a final value of Q that is constant in time and lower than 959 the initial one, whereas $\hat{W}_{\rm rem}$ drives the growth of Q up to an asymptotic 960 value that comes nearer to the initial one, with a rate of convergence ruled by 961 Γ . We remark that, in "standard" remodelling, the parameter Γ is the only 962 quantity that controls the stationary value of Q. 963

Finally, the strongest differences between the two compared models are at the final time of observation and in the relaxation times. Indeed, in the case of "non-standard" remodelling, the energetic contribution \hat{W}_{rem} is predominant in ruling the behaviour of the remodelling variable after the loading ramp, thus when $\partial \hat{W}_{\text{std}}/\partial Q$ tends towards zero, thereby mainly affecting the final state of the system.

In Fig. 7a, we report the axial profile of the circumferential component of the second Piola-Kirchhoff stress tensor *due to the fibres*, i.e.

$$\boldsymbol{S}_{\mathrm{a}} = 2\Phi_{\mathrm{1s}}(\partial \langle \langle \hat{W}_{\mathrm{1a}} \rangle / \partial \boldsymbol{C}),$$

evaluated at $T_{\rm end} = 100 \, \rm s$. As expected, the occurrence of remodelling lowers 970 the stress in the tissue in comparison with the case of no remodelling. We 971 remark, however, that in the case of "non-standard" remodelling the stress 972 behaviour is related to the choice of the boundary conditions imposed on Q. 973 Indeed, the fact that in this work Q is constrained to be equal to $\pi/2$ rad at 974 the upper boundary of the sample (see also Fig. 7b) produces in that zone a 975 value of stress equal to the one obtained in the absence of remodelling. The 976 "standard" remodelling, instead, for which no boundary conditions on Q are 977 required, reduces the stress everywhere in the sample. The deviation is evident 978 in the superficial (upper) zone of the sample, where the mean angle evolves 979 the most (cf. Fig. 7b), and is barely visible in the deep (lower) zone, in which 980 almost no remodelling occurs (see also the trend of Q shown in Fig. 7b). 981

In Fig. 8, we report the axial profile of the mean angle for $t \geq T_{\text{ramp}}$. In 982 particular, by expressing Q as a function of the normalised axial coordinate 983 and time, and recalling the parameter a introduced in (46), we compare the 984 shape of $Q(\xi, t)$ computed for a = 0 with that obtained for $a \neq 0$. For a = 0985 (Fig. 8a), the plot of the mean angle tends to recover its initial shape for 986 $t > T_{\rm ramp}$. For $a \neq 0$ (Fig. 8b), instead, the curves obtained for $t > T_{\rm ramp}$ 987 evolve in time while maintaining a shape similar to the curve determined 988 for $t = T_{\text{ramp}}$. Since the profile of the mean angle is a representation of the 989 pattern of fibre orientation in the sample, we conclude that, as expected, the 990 introduction of a non-vanishing parameter a brings about structural changes 991 that are more pronounced than in the case a = 0. This may be due to the fact 992 that the condition $a \neq 0$ activates the term $\mathcal{A}_0 e^{\hat{\alpha}_W(C)Q} \hat{\alpha}_W(C) \hat{\mathcal{P}}(Q)$ on the 993



Fig. 7 (a) Circumferential component of the anisotropic part of the second Piola-Kirchhoff stress tensor, $(\mathbf{S}_{\rm a})^{22}$ evaluated along the symmetry axis for $t = T_{\rm end}$. (b) Axial profile of the mean angle for $t = T_{\rm end}$. Note that the curves labelled with "AC remodelling" refer to the "non-standard" remodelling and are obtained with a = 0. The units of Γ are J s m⁻³.



Fig. 8 Axial profile of Q for $t \ge T_{\text{ramp}}$ in the case a = 0 (a) and $a = 10^3$ (b). For both cases, we set $\Gamma = 1.0 \cdot 10^4 \text{ J} \text{ s m}^{-3}$.

⁹⁹⁴ right-hand-side of (48b), which gives rise to an additional remodelling force. ⁹⁹⁵ This, in turn, may be responsible for the marked change of the mean angle ⁹⁹⁶ also in the deep zone of the tissue (i.e., for values of ξ closer to zero), where ⁹⁹⁷ otherwise only small changes of the mean angle are observed for a = 0. Indeed, ⁹⁹⁸ when a is set equal to zero, the right-hand-side of (48b) reduces to

$$\frac{\partial \hat{W}}{\partial Q} = \frac{\partial \hat{W}_{\text{std}}}{\partial Q} + \mathcal{A}_0 \frac{\partial \hat{\mathcal{P}}}{\partial Q},\tag{71}$$

and, since $\partial \hat{W}_{\text{std}}/\partial Q$ goes to zero for large times, the remodelling force $\partial \hat{W}/\partial Q$ that remains active also in the limit of large t, i.e., $\mathcal{A}_0 \partial \hat{\mathcal{P}}/\partial Q$, is independent of deformation. This means that, for a = 0, the remodelling becomes asymptotically decoupled from deformation.

¹⁰⁰³ 6 Summary of results and further research

The remodelling considered in our work consists of the reorientation of the collagen fibres of a fibre-reinforced, hydrated soft tissue (e.g. articular cartilage),

in which the fibres are aligned according to a prescribed probability density. 1006 The remodelling process is described through the spatiotemporal evolution of 1007 the mean angle associated with the fibre probability density. The mean angle 1008 is determined by solving the balance of generalised forces presented in (10), in 1009 which the generalised forces \mathcal{R}_{ext} and \mathcal{R}_{int} are said to be external and internal 1010 remodelling forces, respectively. The force \mathcal{R}_{int} is assigned constitutively. To 1011 this end, and motivated by histological observations, we proposed a constitu-1012 tive theory based on the introduction of the remodelling free energy density 1013 $\hat{W}_{\rm rem}$. This takes the spatial resolution of the mean angle explicitly into ac-1014 count, and features the Allen-Cahn term \hat{W}_{AC} , whose minimum configurations 1015 coincide with the mean angles at the lower and upper boundary of the sample. 1016

Our first result is that our model determines the histological profile of the mean angle as the solution of a partial differential equation, rather than by fitting experimental data (see Fig. 2). This result, however, follows also from the choice of the boundary conditions, and a histologically based calibration of the model parameters D_0 and A_0 . We interpreted this result as the manifestation of a spontaneous symmetry breaking, which makes the system pass from a randomly distributed to a non-randomly distributed fibre mean angle.

¹⁰²⁴ A comparison between the theory proposed in this work with that of "stan-¹⁰²⁵ dard" remodelling is reported in Figs. 5, 6, and 7, in which we highlighted the ¹⁰²⁶ influence of \hat{W}_{rem} on the evolution in space and time of the mean angle and ¹⁰²⁷ of the stress distribution within the considered sample of tissue.

Finally, we studied the influence of the parameter a, which features in 1028 the definition of $\hat{\alpha}_W$ (see (46)), on the spatiotemporal evolution of Q. We 1029 remark that, for a = 0, the free energy density \hat{W}_{AC} becomes a function 1030 of Q only, i.e., $\hat{W}_{AC}(Q) = \mathcal{A}_0/(\pi/4)^4 Q^2 (Q - \pi/2)^2$, and is thus invariant 1031 under the discrete symmetry transformation $Q \mapsto \pi/2 - Q$. Such symmetry 1032 manifests itself through the shape of the curves in Fig. 8a. On the contrary, 1033 for $a \neq 0$, $W_{\rm AC}$ loses this discrete symmetry because of the coupling with 1034 the deformation (see (28)). We conclude that our theory of remodelling is 1035 capable of describing the histological profile of the mean angle as the result of 1036 a spontaneous symmetry breaking, which occurs in the tissue independently on 1037 deformation (perhaps, when the tissue is generated) and proposes to interpret 1038 the coupling between the evolution of Q and the deformation as a further 1039 symmetry breaking (this time, however, a non-spontaneous one). 1040

A last remark should be made in regards of the time scales involved in the 1041 considered remodelling process. Such time scales, indeed, are dictated in this 1042 work by the loading history imposed from the outside and, for this reason, they 1043 may appear unnatural. In fact, they represent a situation that is different from 1044 the more natural one in which the characteristic time scale of remodelling is 1045 the result of the coupling of this phenomenon with other processes, like e.g. 1046 growth, and with the deformations and stresses induced by those. Introducing 1047 growth in the description of remodelling presented in this work, and therefore 1048 determining the natural time scales of these phenomena, is one of the objectives 1049 of our studies. 1050

Our long term goal is to employ the approach proposed in our work for 1051 characterising the structural evolution of fibrous tissues also in pathological 1052 situations. For example, collagen orientation in articular cartilage varies due 1053 to several reasons: It has been observed that, in a damaged or aged tissue [65, 1054 66], the fibre orientation is quite far from that in the healthy tissue. In Fig. 1055 9, the numerical results obtained in an unconfined compression test have been 1056 qualitatively compared with the experimental outcomes shown in [65]. The 1057 horizontal lines in the experimental figures mark each of the three zones of 1058 articular cartilage (deep, middle, superficial). We see that, in a stressed and 1059 damaged tissue, these three zones sensibly change, and in particular the deep 1060 zone becomes more extended along the depth of the tissue, while the middle 1061 zone shifts towards the top. A similar axial distribution of the remodelling vari-1062 able can be obtained, by means of the remodelling law (62) presented in this 1063 work, at the end of a loading ramp in an unconfined compression. Naturally, 1064 this result should be enriched by accounting, for example, for the concurrent 1065 mass changes of both the collagen and the matrix, and for the reorganisa-1066 tion of the cells surrounding the fibres during realistic (either physiological or 1067 pathological) loading conditions borne by the tissue. Also this topic is subject 1068 of our current investigations. 1069



Fig. 9 Numerical simulations of an unconfined compression, in the unloaded initial configuration (left) and in the loaded condition at $t = T_{\rm ramp}$ (deformed cylindrical shape on the right), have been qualitatively compared with the experimental results shown in [65]. The experimental observations (reported in the four columns featuring in the figure) correspond to a FT-IRIS image and a polarised light microscopy image (from left to right) directly taken from [65] (open access article). The four columns in the figure are reprinted from [65], Copyright (2005), with permission from Elsevier

1070 Appendix A

To recall the relation between the operators in the physical space and those in the reference configuration of a body, we select an open subset $\mathcal{C} \subset \mathcal{B}$ of the reference configuration and we consider the map $\chi_t \colon \mathcal{C} \to \chi_t(\mathcal{C})$ that, at each time t, embeds \mathcal{C} into the open subset $\chi_t(\mathcal{C}) \subset S$ of the physical space \mathcal{S} . Clearly, it applies that $\chi_t(X) = \chi(X,t)$ for all $X \in \mathcal{C}$ and for all t (cf.

36

Equation (1)). Then, let ${}^{s}f: \chi_{t}(\mathcal{C}) \to \mathbb{R}$ and ${}^{s}u: \chi_{t}(\mathcal{C}) \to TS$ be a scalar and a vector field, respectively, and let $f = {}^{s}f \circ \chi_{t}: \mathcal{C} \to \mathbb{R}$ and $u = {}^{s}u \circ \chi_{t}: \mathcal{C} \to TS$ denote the counterparts of ${}^{s}f$ and ${}^{s}u$ defined over \mathcal{C} . Thus, the identities $f(X) = {}^{s}f(\chi_{t}(X)) = {}^{s}f(x)$ and $u(X) = {}^{s}u(\chi_{t}(X)) = {}^{s}u(x)$ hold true, with $x = \chi_{t}(X) \in \chi_{t}(\mathcal{C})$ and $X \in \mathcal{C}$. Hence, if all the partial derivatives of f and ${}^{s}f$ exist in \mathcal{C} and $\chi_{t}(\mathcal{C})$, respectively, enforcing the chain rule yields

$$\operatorname{Grad} f = [\boldsymbol{F}^{\mathrm{T}} \operatorname{grad}^{\mathrm{s}} f] \circ \chi_{t} \quad \Rightarrow \quad \operatorname{grad}^{\mathrm{s}} f = [\boldsymbol{F}^{-\mathrm{T}} \operatorname{Grad} f] \circ \chi_{t}^{-1}, \quad (72a)$$
$$\operatorname{Grad} \boldsymbol{u} = [(\operatorname{grad}^{\mathrm{s}} \boldsymbol{u}) \circ \chi_{t}] \boldsymbol{F} \quad \Rightarrow \quad (\operatorname{grad}^{\mathrm{s}} \boldsymbol{u}) \circ \chi_{t} = (\operatorname{Grad} \boldsymbol{u})(\boldsymbol{F}^{-1} \circ \chi_{t}). \quad (72b)$$

¹⁰⁸² The divergence of ${}^{s}u$ is given by

$$(\operatorname{div}^{s} \boldsymbol{u}) \circ \chi_{t} = \operatorname{tr}[(\operatorname{grad}^{s} \boldsymbol{u}) \circ \chi_{t}]$$

= tr[(Grad \boldsymbol{u})(\boldsymbol{F}^{-1} \circ \chi_{t})] = (\operatorname{Grad} \boldsymbol{u}) : \boldsymbol{F}^{-\mathrm{T}}. (73)

Note that in (72a), (72b), and (73) the explicit dependence of F on time is omitted but understood, and that, in the definitions of f and u, time t plays the role of a parameter.

Given a differentiable material vector field $U: \mathcal{C} \to T\mathcal{B}$, the divergence of U in \mathcal{C} reads

$$\operatorname{Div} \boldsymbol{U} = \operatorname{tr}[\operatorname{Grad} \boldsymbol{U}]. \tag{74}$$

If ^s \boldsymbol{u} is the flux vector associated with some scalar physical quantity, then the material counterpart of ^s \boldsymbol{u} is defined through the Piola transformation $\boldsymbol{U} = J(\boldsymbol{F}^{-1} \circ \chi_t)\boldsymbol{u}$, with $\boldsymbol{u} = {}^{s}\boldsymbol{u} \circ \chi_t$, and the divergences div ^s \boldsymbol{u} and Div \boldsymbol{U} are related through [41]

$$J(\operatorname{div}^{s} \boldsymbol{u}) \circ \chi_{t} = \operatorname{Div} \boldsymbol{U}.$$

$$(75)$$

In the sequel, the compositions with χ_t and χ_t^{-1} will be omitted for the sake of a lighter notation.

The definitions reported above can be generalised to the computation of 1094 the gradient and divergence of tensor fields of any order (see e.g. [41] for de-1095 tails). If, for example, ^st is a second-order tensor field defined over $\chi_t(\mathcal{C}) \subset S$ 1096 and characterised by contravariant components, its gradient, grad ${}^{s}t$, is a third-1097 order tensor field with two contravariant indices (i.e., those corresponding to 1098 the first pair of indices) and one covariant index (i.e., that individuated by the 1099 direction along which the covariant differentiation is performed), while its di-1100 vergence, div ${}^{s}t$, is the unique vector field satisfying div $({}^{s}t^{T}.h) = (\text{div} {}^{s}t).h$, for 1101 all constant spatial vectors h. In components, div^st reads $(\operatorname{div}^{s} t)^{a} = ({}^{s}t)^{ab}{}_{.b}$, 1102 where the semicolon ";" stands for partial covariant differentiation. 1103

Often, the notation grad ${}^{s}f$ and div ${}^{s}u$ is replaced by grad ${}^{s}f \equiv \nabla {}^{s}f$ and div ${}^{s}u \equiv \nabla \cdot {}^{s}u$ (accordingly, for the material description, one writes Grad $f \equiv$ $\nabla_{R}f$ and Div $U \equiv \nabla_{R} \cdot U$, the subscript "_R" meaning that the differentiation is done in the reference configuration). In this paper, however, for the sake of consistency with the notation adopted in previous works, we prefer to use the ¹¹⁰⁹ symbols "grad" and "div" for the operators in the physical space and "Grad" ¹¹¹⁰ and "Div" for the operators in the reference configuration. Moreover, in the ¹¹¹¹ differential geometric approach that we follow, the symbol nabla, ∇ , is usually ¹¹¹² reserved to a *connection*, i.e., a *covariant derivative*. While ∇ and grad could ¹¹¹³ be used interchangeably, the use of " ∇ -" for div becomes cumbersome as it ¹¹¹⁴ relies on the traditional abuse of notation according to which ∇ is a "vector", ¹¹¹⁵ which does *not* fit with covariant differentiation.

1116 Appendix B

Within a purely mechanical framework (i.e., in the absence of thermal effects), and under the hypothesis that the mass densities of the solid and the fluid phase are constant, the dissipation inequality, written per unit volume of the tissue's reference configuration, can be cast in the form

$$\mathfrak{D}_{0} = -W + \mathbf{P}_{s} : \mathbf{g}\mathbf{F} + \mathbf{P}_{f} : \mathbf{g}\operatorname{Grad}\mathbf{v}_{f} - J\boldsymbol{\pi}_{f}.\mathbf{w} + \mathcal{R}_{int}\dot{Q} + \operatorname{Div}(-T\bar{\boldsymbol{\Omega}}^{\eta}) \ge 0.$$
(76)

Equation (76) is obtained by specialising the theoretical framework developed. 1121 for example, by Hassanizadeh [67], Bennethum et al. [68], and Grillo et al. [22] 1122 to the setting presented in our work. In the definition of \mathfrak{D}_0 , W is the overall 1123 energy density of the solid phase, expressed per unit volume of the reference 1124 configuration and defined in (31a), $P_s: g\dot{F}$ and $P_f: g \operatorname{Grad} v_f$ are the internal 1125 mechanical power densities produced by the agency of the first Piola-Kirchhoff 1126 stress tensors $P_{\rm s}$ and $P_{\rm f}$ on F and ${\rm Grad} v_{\rm f}$, respectively, $J\pi_{\rm f}.w$ is the power 1127 density related to the interaction force between the fluid and the solid phase, 1128 i.e., $\pi_{\rm f}$, which is conjugate to the relative velocity $w = v_{\rm f} - v_{\rm s}$, $\Re_{\rm int} \dot{Q}$ is the 1129 internal power density associated with remodelling, T is absolute temperature, 1130 and $\bar{\mathfrak{Q}}^{\eta}$ is the entropy flux vector. We remark that, since thermal effects are 1131 excluded from the present context, T is here understood as a constant reference 1132 temperature, which provides $T\bar{\mathbf{Q}}^{\eta}$ with the physical units of energy flux vector. 1133 We notice that, in the Classical Thermodynamics of Irreversible Processes, 1134 the entropy flux vector is usually defined by dividing the heat flux vector 1135 by the absolute temperature [69]. Therefore, if this hypothesis is accepted, 1136 there can be no entropy flux vector in a theory in which thermal effects —and, 1137 consequently, the heat flux vector— are disregarded from the outset. However, 1138 within a more general setting, the entropy flux vector of a thermodynamic 1139 theory need not be related a priori to the heat flux vector [55]. In fact, this is 1140 the case studied in our work, which is non-classical in the sense that the free 1141 energy density of the solid phase depends on the gradient of the fibre mean 1142 angle, Q, as well as on Q itself. Hence, if the approach outlined by Jamet 1143 [55] is adopted, one might introduce the entropy flux vector $\bar{\mathbf{\Omega}}^{\eta}$ even in a 1144 purely mechanical framework, in which, thus, the heat flux vector is absent, 1145 and determine a constitutive representation for it. This is, in fact, the path 1146 followed in our work. 1147

¹¹⁴⁸ To show the calculations leading to the definitions of the terms reported ¹¹⁴⁹ in (30a)–(30d), i.e., \mathfrak{D}_{I} , \mathfrak{D}_{II} , \mathfrak{D}_{III} , and \mathfrak{D}_{IV} , we modify (76) as

$$\mathfrak{D} = \mathfrak{D}_{0} + p \left[\Phi_{s} \boldsymbol{F}^{-T} : \dot{\boldsymbol{F}} + (J - \Phi_{s}) \boldsymbol{F}^{-T} : \text{Grad} \boldsymbol{v}_{f} + (J \boldsymbol{g}^{-1} \text{grad} \phi_{f}) \cdot \boldsymbol{w} \right] \ge 0,$$
(77)

where p is pressure, and the sum of the terms in brackets expresses the mass balance law for the system as a whole, i.e.,

$$\Phi_{\rm s} \boldsymbol{F}^{\rm -T} : \dot{\boldsymbol{F}} + (J - \Phi_{\rm s}) \boldsymbol{F}^{\rm -T} : \operatorname{Grad} \boldsymbol{v}_{\rm f} + (J \boldsymbol{g}^{-1} \operatorname{grad} \phi_{\rm f}) \cdot \boldsymbol{w} = 0.$$
(78)

We recall that (78) is obtained by adding together the mass balance laws for the solid and the fluid phase, which, in the case of constant mass densities, can be written as

$$\mathbf{D}_{\mathbf{s}}\phi_{\mathbf{s}} + \phi_{\mathbf{s}}\mathrm{div}\boldsymbol{v}_{\mathbf{s}} = 0, \tag{79a}$$

$$D_{s}\phi_{f} + (grad\phi_{f})\boldsymbol{w} + \phi_{f}div\boldsymbol{v}_{f} = 0, \qquad (79b)$$

and computing the backward Piola transform of the result.

In writing (77), the mass balance law of the mixture as a whole is treated as a constraint of the theory, and the pressure p is thus the Lagrange multiplier associated with it. Moreover, since the terms between brackets in (77) add up to zero, \mathfrak{D} and \mathfrak{D}_0 are numerically equal to each other, although they acquire a rather different meaning. For a discussion on the subject, the Reader is referred to [68].

¹¹⁶² By substituting the expression of \mathfrak{D}_0 in (77), the dissipation inequality ¹¹⁶³ becomes

$$\begin{aligned} \boldsymbol{\mathfrak{D}} &= -\dot{W} + \left[\boldsymbol{P}_{\mathrm{s}} + \boldsymbol{\varPhi}_{\mathrm{s}} p \boldsymbol{g}^{-1} \boldsymbol{F}^{-\mathrm{T}} \right] : \boldsymbol{g} \dot{\boldsymbol{F}} \\ &+ \left[\boldsymbol{P}_{\mathrm{f}} + (J - \boldsymbol{\varPhi}_{\mathrm{s}}) p \boldsymbol{g}^{-1} \boldsymbol{F}^{-\mathrm{T}} \right] : \boldsymbol{g} \operatorname{Grad} \boldsymbol{v}_{\mathrm{f}} \\ &- J [\boldsymbol{\pi}_{\mathrm{f}} - p \boldsymbol{g}^{-1} \operatorname{grad} \boldsymbol{\phi}_{\mathrm{f}}] . \boldsymbol{w} \\ &+ \mathcal{R}_{\mathrm{int}} \dot{Q} + \operatorname{Div} (-T \bar{\boldsymbol{\mathfrak{Q}}}^{\eta}) \geq 0. \end{aligned}$$
(80)

1164 Then, we expand the time derivative of W, thereby obtaining

$$\begin{split} \dot{W} &= \frac{\partial \hat{W}}{\partial \boldsymbol{C}} : \dot{\boldsymbol{C}} + \frac{\partial \hat{W}}{\partial Q} \dot{\boldsymbol{Q}} + \frac{\partial \hat{W}}{\partial \text{Grad}Q} \overline{\text{Grad}Q} \\ &= \frac{\partial \hat{W}}{\partial \boldsymbol{C}} : \dot{\boldsymbol{C}} + \frac{\partial \hat{W}}{\partial Q} \dot{\boldsymbol{Q}} + \frac{\partial \hat{W}}{\partial \text{Grad}Q} \text{Grad}\dot{\boldsymbol{Q}} \\ &= \boldsymbol{F} \left(2 \frac{\partial \hat{W}}{\partial \boldsymbol{C}} \right) : \boldsymbol{g} \dot{\boldsymbol{F}} + \text{Div} \left[\frac{\partial \hat{W}}{\partial \text{Grad}Q} \dot{\boldsymbol{Q}} \right] \\ &+ \left[\frac{\partial \hat{W}}{\partial Q} - \text{Div} \left(\frac{\partial \hat{W}}{\partial \text{Grad}Q} \right) \right] \dot{\boldsymbol{Q}}. \end{split}$$
(81)

Finally, by replacing the right-hand-side of (81) into (80), and grouping together all the terms that multiply the same generalised velocity, we find

$$\mathfrak{D} = \left\{ -F\left(2\frac{\partial\hat{W}}{\partial C}\right) + P_{s} + \Phi_{s}pg^{-1}F^{-T} \right\} : g\dot{F} \\ + \left\{ P_{f} + (J - \Phi_{s})pg^{-1}F^{-T} \right\} : g \operatorname{Grad} v_{f} \\ - J[\pi_{f} - pg^{-1}\operatorname{grad} \phi_{f}] \cdot w \\ + \left\{ \mathcal{R}_{int} - \left[\frac{\partial\hat{W}}{\partial Q} - \operatorname{Div}\left(\frac{\partial\hat{W}}{\partial \operatorname{Grad} Q}\right)\right] \right\} \dot{Q} \\ + \operatorname{Div}\left[-\frac{\partial\hat{W}}{\partial \operatorname{Grad} Q} \dot{Q} - T\bar{\mathfrak{Q}}^{\eta} \right] \ge 0.$$
(82)

Thus, the terms $\mathfrak{D}_{I}, \mathfrak{D}_{II}, \mathfrak{D}_{III}$, and \mathfrak{D}_{IV} can be identified by comparing (82) 1167 with (30a)–(30d). In principle, \mathfrak{D}_{I} accounts for the dissipative stresses asso-1168 ciated with the solid and the fluid phase, respectively. However, since in our 1169 work the solid phase is assumed to be hyperelastic, and the fluid is assumed 1170 to be macroscopically inviscid, neither the solid nor the fluid phase feature 1171 a dissipative stress. Hence, \mathfrak{D}_{I} must vanish identically. The term \mathfrak{D}_{II} is the 1172 dissipation due to the solid-fluid interactions. In fact, the brackets multiplying 1173 w define the dissipative part of the interaction force density $\pi_{\rm f}$, which leads to 1174 Darcy's law. Analogously, \mathfrak{D}_{III} consists of the dissipation related to the process 1175 of remodelling, and the coefficient of Q determines the dissipative part of the 1176 internal remodelling generalised force \mathcal{R}_{int} . Finally, \mathfrak{D}_{IV} is assumed to vanish 1177 in the present context, thereby defining the entropy flux vector $\mathbf{\hat{\Omega}}^{\eta}$. 1178

We emphasise that the framework within which the dissipation inequality 1179 is studied in our work is based on the hypothesis of validity of Darcy's law for 1180 the description of the fluid filtration velocity. Moreover, neither the dissipa-1181 tive effects related to the mixture viscosity [70] nor those connected with the 1182 microstructure viscosity of the considered medium [70] are taken into account. 1183 These, however, can be relevant in the poroelastic approach to bone structure 1184 developed in [70]. In addition, for increasing magnitude of the tissue's per-1185 meability, also a possible deviation from the flow regime predicted by Darcy's 1186 law can be appreciable. Indeed, when this is the case, the Brinkman correction 1187 should be included into the model [70]. 1188

1189 Acknowledgements We would like to thank Dr. Lorenzo Tentarelli for useful discussions.

¹¹⁹⁰ In Memoriam

¹¹⁹¹ In memory of our master, Prof. Gaetano Giaquinta (1945–2016), who inspired ¹¹⁹² this work back in 2004, by suggesting the use of the Ginzburg-Landau energy.

1193

¹¹⁹⁴ Compliance with Ethical Standards

¹¹⁹⁵ The authors declare that they have no conflict of interest.

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42

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