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EXTENDED CONCEPT OF REPRESENTATIVE DIRECTIONS TO DESCRIBE INELASTIC BEHAVIOUR OF ELECTROSPUN POLYMERS

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Abstract. The concept of representative directions allows one to generalize one-dimensional uniaxial material models to more general constitutive equations, suitable for arbitrary multi-axial loading scenarios. The procedure preserves the thermodynamic consistency and the resulting material model satisfies the principle of objectivity. In the current paper, the concept is modified by the introduction of new kinematics. Some features of the resulting constitutive equations as well as the applicability of the extended concept to real materials are discussed. For demonstration purposes, the plastic behaviour of an electrospun polymer is modelled under large strain non-monotonic loading.

1 INTRODUCTION

The development of advanced material models is a multifaceted task, since a number of requirements must be met. First, the developed model must satisfy the general principles of constitutive mechanics, like objectivity, thermodynamic consistency, and preservation of material symmetries. Second, the model must describe the real stress response with a sufficient accuracy for a broad spectrum of loading conditions. Third, a robust identification of material parameters must be possible based on a limited number of experiments. Finally, the model must allow for an efficient and reliable numerics. At the conceptual stage of constitutive modelling one may develop a simplified one-dimensional version of the model which is suitable for uniaxial loading scenarios only. Classical examples are the uniaxial Hooke law in elasticity and the Masing rule in cyclic plasticity [12]. Unfortunately, these one-dimensional laws can not be used for the analysis of general application involving multi-axial loading conditions. To generalize the one-dimensional model, a number of techniques were developed. The current paper focuses on the concept of representative directions (see [16, 4, 15, 5]). It is based on the assumption that for each material particle

the stress power is equal to the sum of stress powers of individual material directions (see Section 2.1). Dealing with one-dimensional laws of hyperelastic type, this assumption is equivalent to the "angular integrations approach" from [9] (see also [3], [10], [7], [11], [8]). In the hyperelastic case the overall free energy is assumed as a sum of energies of individual material directions. In order to obtain a stress tensor as a function of the strain history, an integration over all possible directions is required which is equivalent to the integration over a unit sphere (semi-sphere). Other approaches which also involve the integration over a unit sphere are the micro-plane approach from [2] and the micro-sphere approach [13], [14], [6].

In the current contribution, a modified version of the concept of representative directions is discussed. The main difference from the classical concept lies in a new definition of the strain for each representative direction. Just as for the original approach, the extended concept preserves the thermodynamic consistency and objectivity. It is shown that if the representative directions are equipped with the one-dimensional Hooke law, the new concept yields the well-known Hencky material. The applicability of the concept to real materials is demonstrated; the behaviour of an electrospun polymer subjected to non-monotonic loading is modelled.

2 CONCEPT OF REPRESENTATIVE DIRECTIONS

2.1 Classical method: C-approach

For simplicity, all the considerations are restricted to incompressible material behaviour.

$$\det(\mathbf{F}) \equiv 1 \;\Rightarrow\; \det \mathbf{C} \equiv 1 \;\Rightarrow\; \dot{\mathbf{C}} : \mathbf{C}^{-1} = 0. \tag{1}$$

By $\mathbf{C}(t)$, $t \in [0, T]$ we denote the local deformation history described in terms of the right Cauchy-Green tensor. Assume that each material particle consists of N fibres. In this subsection the term "fibre" will be used along with the term "representative material direction". For each fibre we introduce a unit vector $\mathbf{e}_\alpha$ ($\alpha = 1, 2, ..., N$) which is directed along the fibre in the reference configuration. The stretch of each fibre α is computed through

$$\lambda_\alpha = \sqrt{\overline{\mathbf{C}} : (\mathbf{e}_\alpha \otimes \mathbf{e}_\alpha)}, \quad \overline{\mathbf{C}} = (\det \mathbf{C})^{-1/3} \cdot \mathbf{C}. \tag{2}$$

Assume that a one-dimensional uniaxial constitutive law is given, which provides uniaxial true stress $\sigma_\alpha(t)$ as a function of the stretch history $\lambda_\alpha(t')$, $t' \in [0, t]$.

Since the true stress σ_α is power conjugate to the true strain $\varepsilon_\alpha = \ln(\lambda_\alpha)$ in incompressible case, $\sigma_\alpha \cdot \dot{\varepsilon}_\alpha$ equals the stress power of the fibre. By $\tilde{\mathbf{T}}$ we denote the second Piola-Kirchhoff stress tensor. We assume that the stress power of the material is equal to the average of individual stress powers of the fibres:

$$\tilde{\mathbf{T}} : \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{N}\sum_{\alpha=1}^{N} \sigma_\alpha \cdot \frac{d}{dt}(\ln \lambda_\alpha), \text{ for all } \dot{\mathbf{C}}, \text{ such that } \dot{\mathbf{C}} : \mathbf{C}^{-1} = 0. \tag{3}$$

Obviously,

$$\dot{\varepsilon}_\alpha = \frac{d}{dt}(\ln \lambda_\alpha) = \frac{1}{2\lambda_\alpha^2}(\mathbf{e}_\alpha \otimes \mathbf{e}_\alpha) : \dot{\overline{\mathbf{C}}}. \tag{4}$$

Combining this equation with (3) we obtain the second Piola-Kirchhoff stress in the following form

$$\tilde{\mathbf{T}} = \frac{1}{N}\sum_{\alpha=1}^{N}\frac{\sigma_\alpha}{\lambda_\alpha^2}(\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha) + \tilde{p}\mathbf{C}^{-1}, \tag{5}$$

where $\tilde{p}\in\mathbb{R}$ is a real number; the term $\tilde{p}\mathbf{C}^{-1}$ naturally appears due to the incompressibility constraint $\dot{\mathbf{C}}:\mathbf{C}^{-1}=0$. The method based on (5) will be called C-approach, since the stretches λ_α of individual fibres are calculated using the right Cauchy-Green tensor $\mathbf{C}$.

2.2 Extended method: H-approach

By $\mathbf{H} := \frac{1}{2}\ln(\mathbf{C})$ we denote the referential Hencky strain measure (logarithmic strain tensor). Within the extended approach, we abandon the straightforward definition of the stretch previously adopted for individual directions. A generalized true strain pertaining to certain direction is now defined using $\mathbf{H}$:

$$\varepsilon_\alpha := \mathbf{H}^{\mathrm{D}} : (\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha) = \mathbf{H} : (\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha)^{\mathrm{D}}. \tag{6}$$

Now the term "representative direction" is not identical to the term "fibre" in the common sense since material fibres and representative directions experience different strains.

The generalized true strain rate for each representative direction equals

$$\dot{\varepsilon}_\alpha = (\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha)^{\mathrm{D}} : \dot{\mathbf{H}} = (\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha)^{\mathrm{D}} : \frac{1}{2}\frac{\partial\ln(\mathbf{C})}{\partial\mathbf{C}} : \dot{\mathbf{C}}. \tag{7}$$

Since the fourth-rank tensor $\frac{\partial\ln(\mathbf{C})}{\partial\mathbf{C}}$ exhibits the full symmetry, we have

$$\dot{\varepsilon}_\alpha = \frac{1}{2}\Big(\frac{\partial\ln(\mathbf{C})}{\partial\mathbf{C}} : (\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha)^{\mathrm{D}}\Big) : \dot{\mathbf{C}}. \tag{8}$$

Just as in the previous subsection, assume that σ_α is the uni-axial stress of a fibre-like object and σ_α is power-conjugate to the generalized true strain ε_α. Following the general concept, we assume that the stress power per unit volume of the material equals the average of individual stress powers of representative directions:

$$\tilde{\mathbf{T}} : \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{N}\sum_{\alpha=1}^{N}\sigma_\alpha\cdot\dot{\varepsilon}_\alpha, \text{ for all } \dot{\mathbf{C}}, \text{ such that } \dot{\mathbf{C}}:\mathbf{C}^{-1}=0. \tag{9}$$

Combining this with (8), we obtain the second Piola-Kirchhoff stress in the form

$$\tilde{\mathbf{T}} = \frac{\partial\ln(\mathbf{C})}{\partial\mathbf{C}} : \Big(\frac{1}{N}\sum_{\alpha=1}^{N}\sigma_\alpha(\mathbf{e}_\alpha\otimes\mathbf{e}_\alpha)^{\mathrm{D}}\Big) + \tilde{p}\mathbf{C}^{-1}. \tag{10}$$

Here, just as in the classical concept, $\tilde{p}\mathbf{C}^{-1}$ appears due to the incompressibility constraint; this term stands for the unknown hydrostatic component of the stress tensor. Since the

generalized true strains of individual representative directions are computed now using the Hencky strain, we call this method H-approach.

In a general plastic (viscoplastic) case, $\sigma_\alpha(t)$ depends on the strain history $\varepsilon_\alpha(t')$, $t' \leq t$:

$$\sigma_\alpha(t) = \sigma(\varepsilon_\alpha(t'), t' \leq t). \tag{11}$$

Note that in both approaches the second Piola-Kirchhoff stress $\tilde{\mathbf{T}}$ depends on the history of the right Cauchy-Green tensor $\mathbf{C}$. Therefore, the objectivity constraint is a priory satisfied. Another advantage of both methods is the automatic preservation of thermodynamic consistency, if the used one-dimensional material laws are thermodynamically consistent as well (for the C-approach it was already shown in [15]).

3 SPECIAL CASE OF LINEAR ELASTICITY

In this section we analyze the performance of the H-approach when the one-dimensional material behaviour is governed by the linear relation between the generalized true stress σ_α and the corresponding true strain ε_α:

$$\sigma_\alpha = E \cdot \varepsilon_\alpha. \tag{12}$$

Here, $E \geq 0$ is the Young modulus of generalized fibres (representative directions). For each direction we introduce the corresponding free energy function ψ_α. In order to ensure that the stress power $\sigma_\alpha \cdot \dot{\varepsilon}_\alpha$ equals $\dot{\psi}_\alpha$ for arbitrary processes, it is necessary and sufficient to assume that

$$\sigma_\alpha = \frac{d\psi_\alpha(\varepsilon_\alpha)}{d\varepsilon_\alpha}, \quad \psi_\alpha(\varepsilon_\alpha) = \frac{1}{2} E \varepsilon_\alpha^2. \tag{13}$$

In other words, the linear relation (12) is of hyperelastic type. Next, recall that the overall stress power equals the average of stress powers of representative directions. Thus, we obtain for all isochoric deformation processes

$$\tilde{\mathbf{T}} : \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{N}\sum_{\alpha=1}^{N} \sigma_\alpha \cdot \dot{\varepsilon}_\alpha = \frac{1}{N}\sum_{\alpha=1}^{N} \dot{\psi}_\alpha = \dot{\psi}, \text{ where } \psi = \frac{1}{N}\sum_{\alpha=1}^{N} \psi_\alpha. \tag{14}$$

Thus, the H-approach yields in this case a hyperelastic material with the free energy

$$\psi = \frac{1}{N}\sum_{\alpha=1}^{N} \psi_\alpha = \frac{1}{N}\sum_{\alpha=1}^{N} \frac{1}{2} E \varepsilon_\alpha^2 = \frac{E}{2N}\sum_{\alpha=1}^{N} (\mathbf{H}^{\mathrm{D}} : (\mathbf{e}_\alpha \otimes \mathbf{e}_\alpha))^2. \tag{15}$$

Assume that the representative directions $\mathbf{e}_\alpha$ are (nearly) equally spaced and the number of directions is large. Thus, in the limiting case as $N \to \infty$, the right-hand side of (15) is an *isotropic quadratic form* of $\mathbf{H}^{\mathrm{D}}$. Using the representation theorem for isotropic quadratic forms, and taking into account that $\mathrm{tr}(\mathbf{H}^{\mathrm{D}}) = 0$, the free energy simplifies to

$$\psi = \frac{\mu}{2}\mathbf{H}^{\mathrm{D}} : \mathbf{H}^{\mathrm{D}}, \tag{16}$$

where μ is a suitable constant (shear modulus). Thus, in the special case of linear elasticity, the H-approach yields the well-known hyperelasticity of Hencky type, where the free energy is a quadratic function of $\mathbf{H}^{\mathrm{D}}$.

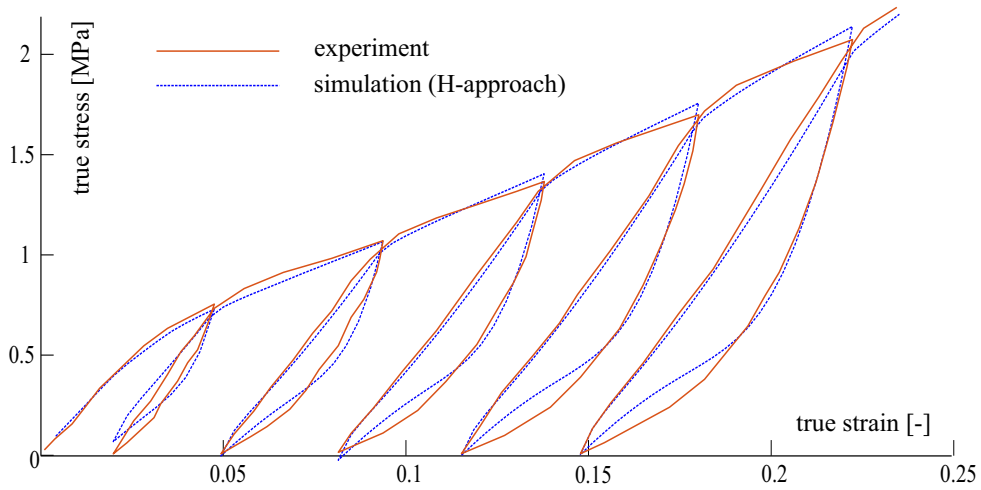

Figure 1: Experimental results taken from [17] on the uniaxial deformation of the electrospun material and corresponding simulation results obtained using the H-approach.

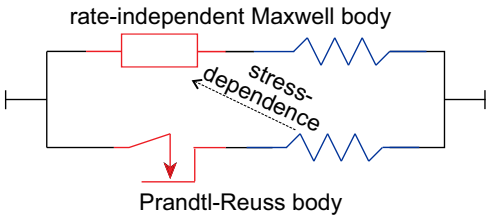

Figure 2: Rheological explanation of the uniaxial material model, used to capture the mechanical response of the electrospun polymer.

4 ELECTROSPUN POLYMER IN THE PLASTIC RANGE

Here we test the performance of the H-approach in terms of a special one-diemensional plasticity model. As a motivation for the studies we start from the experimental results presented in [17] dealing with a uniaxial deformation of an electrospun polymer, see Fig. 1. Clearly, the stress response of the analyzed material is inelastic with a complex form of the hysteresis loops.

As a vivid explanation of the underlying uniaxial material model we use the rheological device presented in Fig. 2. This one-dimensional rheological model consists of the friction element which is attached in series to an elastic spring. We call the obtained elasto-plastic element one-dimensional Prandtl-Reuss body. Next, the rate-independent dashpot (shown as a box in the figure) is attached in series to another elastic spring. The obtained element is referred to as the rate-independent Maxwell body. The overall uniaxial model is a parallel connection of the Prandtl-Reuss body and the rate-independent Maxwell body. Denote by σ_{PR} and σ_{M} the stresses which act in these bodies. Thus, we have

$$\sigma = \sigma_{\mathrm{PR}} + \sigma_{\mathrm{M}}. \tag{17}$$

The behaviour of the Prandtl-Reuss body is governed by the following relations:

$$\sigma_{\mathrm{PR}} = E_{\mathrm{PR}} \cdot \varepsilon_{\mathrm{e}}, \tag{18}$$

$$\varepsilon_{\mathrm{e}} = \varepsilon - \varepsilon_{\mathrm{p}}, \tag{19}$$

$$\dot{\varepsilon}_{\mathrm{p}} = |\dot{\varepsilon}_{\mathrm{p}}| \cdot \mathrm{sign}(\sigma_{\mathrm{PR}}). \tag{20}$$

A linear isotropic hardening is considered:

$$|\sigma_{\mathrm{PR}}| \leq \ K_0 + \gamma s. \tag{21}$$

Here, E_{PR}, K_0, and γ are material parameters; s is the accumulated plastic strain:

$$s(t) = \int_{\tilde{t}=0}^{\tilde{t}=t} |\dot{\varepsilon}_{\mathrm{p}}| d\tilde{t}. \tag{22}$$

Next, we use the following viscous flow rule

$$|\dot{\varepsilon}_{\mathrm{p}}| = \frac{1}{\eta}\big\langle |\sigma_{\mathrm{PR}}| - (K_0 + \gamma s)\big\rangle, \tag{23}$$

where η is a material parameter (viscosity); $\langle x\rangle = \max(0, x)$ is the Macaulay bracket. The rate-independent case is restored as $\eta \to 0$.

The equations of the rate-independent Maxwell body are the same as for the classical rate-dependent one, the only difference is that the physical time t is replaced by the monotonically increasing accumulated strain. Thus we have

$$\dot{\sigma}_{\mathrm{M}} = E_{\mathrm{M}} \cdot \dot{\varepsilon} - b \cdot |\dot{\varepsilon}| \cdot \sigma_{\mathrm{M}}, \tag{24}$$

where $E_{\mathrm{M}} \geq 0$ is a fixed parameter, $b \geq 0$ is a process-dependent "viscosity". In this study we assume

$$b = \frac{b_0}{|\sigma_{\mathrm{PR}}|^2 + b_1}, \tag{25}$$

where b_0 and b_1 are fixed positive parameters. Thus, the generalized viscosity depends on the stresses from the Prandtl-Reuss body. Simple and efficient numerical algorithms can be constructed for the one-dimensional model (17) – (25).

Recall that within the H-approach σ_α and ε_α are (generalized) true stresses and strains. Unfortunately, computations using the uniaxial model (17) – (25) where σ and ε are interpreted as true stresses and strains were not satisfying. The accuracy of the material modelling can be improved when σ and ε which appear in (17) – (25) are seen as engineering stresses and strains. Therefore, the following (geometric) pre- and post-processing is used here: $\varepsilon := e^{\varepsilon_\alpha} - 1$, $\sigma_\alpha := \sigma(1 + \varepsilon)$.

A total number of 100 (nearly) equally spaced directions is used for testing purposes. The unknown material parameters are identified by fitting the predicted stress response to the available experimental data. The fitted parameters are listed Table 1. As is seen from Fig. 1, the H-approach to the concept of representative direction reproduces the real material behaviour with a good accuracy.

Table 1: Identified material constants

K_0 [MPa]	γ [MPa]	η [MPa s]	E_{PR} [MPa]	E_{M} [MPa]	b_0 [MPa^2]	b_1 [MPa^2]
1.38	28.9	0.0	82.5	179.9	1258.0	0.618

5 CONCLUSION

Within the classical C-approach the individual directions can be understood as fibres, whose stretch is naturally defined by (2). Unfortunately, this simple interpretation is lost for the generalized H-approach, since a more complex kinematics is used to define the strain of individual directions, see Eq. (6). At the same time, this assumption is a part of an extended approach which respects the thermodynamic consistency and objectivity. It is shown that in the case of a linear relation between true stresses and strains in the one-dimensional model, the H-approach yields the well-known Hencky material. It is a hyperelastic material with the strain energy given by a quadratic function of the referential Hencky strain. The applicability of the H-approach to a real material is tested. The mechanical behaviour of the electrospun polymer is rendered with a good accuracy.

In the follow-up paper, second order effects like the Swift and Poynting will be discussed and the modelling of initial isotropy will be thoroughly analyzed.

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REFERENCES

[1] Idelsohn, S.R. and Oñate, E. Finite element and finite volumes. Two good friends. *Int. J. Num. Meth. Engng.* (1994) **37**:3323–3341.

[2] Bažant, Z.P. and Oh, B.H. Microplane model for progressive fracture of concrete and rock. *Journal of Engineering Mechanics* (1985) **111**:559–582.

[3] Federico, S. and Herzog, W. Towards ananalytical model of soft biological tissues. *Journal of Biomechanics* (2008) **41**:3309–3313.

[4] Freund, M. and Ihlemann, J. Generalization of one-dimensional material models for the finite element method. *ZAMM* (2010) **90**(5):399–417.

[5] Freund, M., Shutov, A.V. and Ihlemann, J. Simulation of distortional hardening by generalizing a uniaxial model of finite strain viscoplasticity. *International Journal of Plasticity* (2012) **36**:113–129.

[6] Göktepe, S. and Miehe, C. A micro-macro approach to rubber-like materials. Part III: The micro-sphere model of anisotropic Mullins-type damage. *Journal of the Mechanics and Physics of Solids* (2005) **53**:2259–2283.

[7] Holzapfel, G.A. and Ogden, R.W. On the tensionecompression switch in soft fibrous solids. *European Journal of Mechanics A/Solids* (2015) **49**:561–569.

[8] Holzapfel, G.A. and Ogden R.W. Comparison of two model frameworks for fiber dispersion in the elasticity of soft biological tissues. *European Journal of Mechanics A/Solids* (2017) **66**:193–200.

[9] Lanir, Y. Constitutive equations for fibrous connective tissues. *Journal of Biomechanics* (1983) **16**:1–12.

[10] Lanir, Y. and Namani, R. Reliability of structure tensors in representing soft tissues structure. *Journal of The Mechanical Behavior of Biomedical Materials* (2015) **46**:222–228.

[11] Li, K., Ogden, R.W. and Holzapfel, G.A. Computational method for excluding fibers under compression in modeling soft fibrous solids. *European Journal of Mechanics A/Solids* (2016) **57**:178–193.

[12] Masing, G.E. Eigenspannungen und Verfestigung beim Messing. *Proc. 2nd Int. Conf. Applied Mech., Zürich* (1926), 332–335.

[13] Miehe, C., Göktepe, S. and Lulei, F. A micro-macro approach to rubber-like materials. Part I: the non-a,ne micro-sphere model of rubber elasticity. *Journal of the Mechanics and Physics of Solids* (2004) **52**:2617–2660.

[14] Miehe, C. and Göktepe, S. A micro-macro approach to rubber-like materials. Part II: The micro-sphere model of finite rubber viscoelasticity. *Journal of the Mechanics and Physics of Solids* (2005) **53**:2231–2258.

[15] Naumann, C. and Ihlemann, J. Thermomechanical material behaviour within the concept of representative directions. *In: Jerrams, S., Murphy, N. (Eds.), Constitutive Models for Rubber VII. Balkema, Leiden* (2011) 107–112.

[16] Pawelski, H., *Eigenschaften von Elastomerwerkstoffen mit Methoden der statistischen Physik*. Shaker-Verlag (1998).

[17] Wong, D., Andriyana, A., Ang, B.C. and Verron, E. Surface morphology and mechanical response of randomly oriented electrospun nanofibrous membrane. *Polymer Testing* (2016) **53**:108–115.