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In this version, the tensor order of a variable equals the number of underlines beneath it.

Caveats concerning conjugate stress and strain measures for frame indifferent anisotropic elasticity

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Summary. Small-distortion constitutive laws are often extemporaneously generalized to large deformations by merely applying them in the unrotated material frame or, equivalently, by using polar rates. This approach does render the resulting constitutive model indifferent to large superimposed rigid rotations, but it may lead to incorrect predictions for both the magnitude and direction of stress whenever there is significant material distortion. To demonstrate this claim, an exact large-deformation solution is derived for the stress in an idealized fiber-reinforced composite. This example shows that the Cauchy tangent stiffness tensor (corresponding to the conjugate pair of Cauchy stress and the symmetric part of the velocity gradient) must evolve in both magnitude and direction whenever the material distorts. Volume changes necessarily lead to a loss of major-symmetry of this Cauchy tangent stiffness tensor, which can be rectified by instead using specific or Kirchhoff stress. A previous work that correctly pointed out the need for the Cauchy stiffness tensor to distort is shown to have overlooked an additional contribution from the rate of distortion. Some of the anomalous properties of the Cauchy stiffness tensor are eradicated by instead using the second Piola-Kirchhoff stress or, equivalently, convected coordinates. Such an approach, however, demands accurate measurements of large-distortion material response, not only to obtain physically realistic results, but also to avoid potential instabilities in numerical computations.

1 Introduction

This paper explores some counterexamples that remind us why *a sensible large-distortion (or even moderate-distortion) constitutive law cannot be constructed from a small-distortion law by merely applying the small-distortion law in the unrotated configuration.* Satisfying the principle of material frame indifference does not guarantee an accurate large-deformation constitutive law. This fact is, of course, well-known and acknowledged within the academic research community (especially in the fluid mechanics literature), but is nevertheless occasionally ignored amidst pressures to solve complete problems. Alternative stress-strain measures or approaches such as convected coordinates can improve results, but can be difficult to implement and still do not liberate the researcher from actually measuring material response at large distortions.

Within the solids field, popular conjugate stress and strain rate measures are the Cauchy stress $\underset{\sim}{\sigma}$ and the symmetric part of the velocity gradient, **D**. To satisfy the principle of material frame indifference, relations involving these two variables are often phrased in terms of the “unrotated” Cauchy stress,

$$\bar{\sigma}_{ij} \equiv R^T_{ip} R^T_{jq} \sigma_{pq} \quad , \tag{1}$$

and the “unrotated” symmetric part of the velocity gradient,

$$\overline{D}_{ij} \equiv R^T_{ip} R^T_{jq} D_{pq} \ . \tag{2}$$

Here, repeated indices are summed from 1 to 3, a superscript "T" denotes the transpose (i.e., $R^T_{ip} = R_{pi}$), and $\underset{\approx}{\mathbf{R}}$ is the proper rotation from the polar decomposition of the deformation gradient $\underset{\approx}{\mathbf{F}}$,

$$\underset{\approx}{\mathbf{F}} = \underset{\approx}{\mathbf{R}} \bullet \underset{\approx}{\overline{\mathbf{V}}} \qquad (i.e., \ F_{ij} = R_{ik} \overline{V}_{kj}), \tag{3}$$

where $\underset{\approx}{\overline{\mathbf{V}}}$ (more commonly denoted $\underset{\approx}{\mathbf{U}}$) is the symmetric positive-definite "right" stretch. A deformation involves "small distortions" if $\underset{\approx}{\overline{\mathbf{V}}} \approx \underset{\approx}{\mathbf{I}}$. A deformation is "arotational" if $\underset{\approx}{\mathbf{R}} = \underset{\approx}{\mathbf{I}}$.

Throughout this paper, an overbar denotes an operation that "unrotates" the basis of any spatial tensor back to the reference configuration, leaving the components unchanged. Thus,

$$\textit{If } \underset{\sim}{\mathbf{w}} \textit{ is a vector,} \quad \overline{w}_i = R^T_{ip} w_p . \tag{4}$$

$$\textit{If } \underset{\approx}{\mathbf{A}} \textit{ is a second-order tensor,} \quad \overline{A}_{ij} = R^T_{ip} R^T_{jq} A_{pq} . \tag{5}$$

$$\textit{If } \underset{\approx\approx}{\mathbf{Y}} \textit{ is a fourth-order tensor,} \quad \overline{Y}_{ijkl} = R^T_{ip} R^T_{jq} R^T_{kr} R^T_{ls} Y_{pqrs} , \tag{6}$$

and so on. The polar rate $\overset{\circ}{\mathbf{A}}$ of any second-order tensor $\mathbf{A}$ is defined by

$$\overset{\circ}{\underset{\approx}{\mathbf{A}}} \equiv \dot{\underset{\approx}{\mathbf{A}}} - \underset{\approx}{\Omega} \bullet \underset{\approx}{\mathbf{A}} + \underset{\approx}{\mathbf{A}} \bullet \underset{\approx}{\Omega} \ , \tag{7}$$

where $\underset{\approx}{\Omega} \equiv \dot{\underset{\approx}{\mathbf{R}}} \bullet \underset{\approx}{\mathbf{R}}^T$ is the polar spin and a superposed dot denotes the usual material rate. The more general definition of the polar rate (applicable for tensors of *any* order),

$$\overline{\overset{\circ}{\underset{\approx}{\mathbf{A}}}} = \dot{\overline{\underset{\approx}{\mathbf{A}}}} , \tag{8}$$

may be used to prove that any linear constitutive relation phrased in terms of polar rates of spatial tensors is equivalent to the same relation phrased in terms of material rates of the associated unrotated tensors.

The second Piola-Kirchhoff (PK2) stress $\underset{\approx}{\bar{\mathbf{s}}}$ is a commonly-used alternative stress measure defined by $\underset{\approx}{\bar{\mathbf{s}}} \equiv J \underset{\approx}{\mathbf{F}}^{-1} \bullet \underset{\approx}{\sigma} \bullet \underset{\approx}{\mathbf{F}}^{-T}$. In indicial notation,

$$\bar{s}_{ij} \equiv J F^{-1}_{ip} F^{-1}_{jq} \sigma_{pq} = J \overline{V}^{-1}_{ip} \overline{V}^{-1}_{jq} \bar{\sigma}_{pq} \ , \tag{9}$$

where the Jacobian J is the ratio of the initial mass density ρ_o to final density ρ:

$$J \equiv \det(\underset{\approx}{\mathbf{F}}) = \frac{\rho_o}{\rho} . \tag{10}$$

The Lagrange strain $\underset{\approx}{\bar{\varepsilon}}$, defined by

$$\underset{\approx}{\bar{\varepsilon}} \equiv \frac{1}{2}(\underset{\approx}{\mathbf{F}}^T \bullet \underset{\approx}{\mathbf{F}} - \underset{\approx}{\mathbf{I}}) = \frac{1}{2}(\underset{\approx}{\overline{\mathbf{V}}} \bullet \underset{\approx}{\overline{\mathbf{V}}} - \underset{\approx}{\mathbf{I}}) , \tag{11}$$

is conjugate to the PK2 stress $\underset{\approx}{\bar{\mathbf{s}}}$.

The unrotated symmetric part of the velocity gradient (Eq. (2)) is related to the stretching rate $\dot{\overline{\mathbf{V}}}$ and the Lagrange strain rate $\underset{\approx}{\dot{\bar{\varepsilon}}}$ by

$$\underset{\approx}{\overline{\mathbf{D}}} = \frac{1}{2}(\underset{\approx}{\dot{\overline{\mathbf{V}}}} \bullet \underset{\approx}{\overline{\mathbf{V}}}^{-1} + \underset{\approx}{\overline{\mathbf{V}}}^{-1} \bullet \underset{\approx}{\dot{\overline{\mathbf{V}}}}) = \underset{\approx}{\overline{\mathbf{V}}}^{-1} \bullet \underset{\approx}{\dot{\bar{\varepsilon}}} \bullet \underset{\approx}{\overline{\mathbf{V}}}^{-1} . \tag{12}$$

Constitutive laws phrased in terms of the PK2 stress $\underset{\approx}{\bar{\mathbf{s}}}$ and the Lagrange strain $\underset{\approx}{\bar{\varepsilon}}$ satisfy the principle of material frame indifference, as do those that use the unrotated Cauchy stress $\underset{\approx}{\bar{\sigma}}$ and unrotated rate-of-deformation $\underset{\approx}{\overline{\mathbf{D}}}$, though the two approaches do not give identical results. Importantly, *merely satisfying the principle of material frame indifference is not sufficient to make a model sensible for high-distortion problems such as penetration*. Many so-called large-deformation constitutive laws are in fact valid only for large *rotations*, not large *distortions*. When users or developers apply such a model beyond its applicability, the model itself might be wrongly blamed for the incorrect results. More seriously, material constants might be inappropriately "tuned" to match experimental results for deformations that lie beyond the model's capability, thereby marring the model's credibility for any other loading paths.

To illustrate these points, an *exact* stress-strain relation will be derived for a microstructure consisting of thin idealized fibers embedded in a negligibly stiff matrix (air). For very thin fibers, the Cauchy stress must always be uniaxial in the fiber direction. However, even for pure stretch deformations, the fiber direction generally changes with time, so the *rate* of the unrotated Cauchy stress is not uniaxial. This directional rate effect (negligible for small distortions without residual stress) is rarely captured in modern large-deformation constitutive laws and can be naturally accommodated by phrasing the constitutive law in terms of the PK2 stress, though the *magnitude* of the result must still be governed by high-distortion experimental data.

For our fibers-in-air example, $\dot{\bar{\sigma}}$ will be shown to be linear in $\bar{\mathbf{D}}$. That is, there does exist a fourth-order tensor $\bar{\mathbf{L}}$ such that $\dot{\bar{\sigma}}_{ij} = \bar{L}_{ijpq}\bar{D}_{pq}$. However, we show here that $\bar{\mathbf{L}}$ will not be major-symmetric (that is, $\bar{L}_{ijpq} \neq \bar{L}_{pqij}$) if there are dilatation rates. Major symmetry may be recovered, however, if the stress measure is replaced by the thermodynamically consistent *specific* stress (stress divided by density), or equivalently by the Kirchhoff stress, $J\bar{\sigma}$ (which may explain its increased use in modern constitutive models).

2 Exact solution for an idealized fiber-reinforced material

Consider a material consisting of stiff fibers uniformly distributed in a very weak matrix (air). *Single* fibers are presumed well-characterized. That is, if a single fiber is stretched so that its current length divided by its initial length is λ, then the force in that fiber is given by some *known* function $F(\lambda)$ satisfying $F(1)=0$.

Suppose all the fibers have an initial orientation parallel to a unit vector $\bar{\mathbf{M}}$, and they are distributed uniformly with ν_o fibers per unit *initial* cross-sectional area. Then the representative volume element sketched in Fig. 1 contains a total of $\nu_o A_o$ fibers. A homogeneous deformation $\mathbf{F}$ will distort those fibers to a new orientation parallel to

$$\mathbf{m} \equiv \mathbf{F} \bullet \bar{\mathbf{M}} \ . \tag{13}$$

The fiber stretch λ is just the magnitude of $\mathbf{m}$:

$$\lambda \equiv \sqrt{\bar{\mathbf{M}} \bullet \mathbf{F}^T \bullet \mathbf{F} \bullet \bar{\mathbf{M}}} = \sqrt{\mathbf{m} \bullet \mathbf{m}} \ . \tag{14}$$

In Fig. 1, the initial cross-sectional area A_o has a unit normal $\bar{\mathbf{N}}=\bar{\mathbf{M}}$. By Nanson's relation [1], this initial area deforms to a new orientation parallel to

$$\mathbf{n} \equiv \mathbf{F}^{-T} \bullet \bar{\mathbf{N}} \ . \tag{15}$$

Also by Nanson's relation, the magnitude of the deformed area is $A = JA_o|\mathbf{n}|$. Figure 1 depicts the deformed element as seen in the plane containing $\mathbf{m}$ and $\mathbf{n}$ where it is clear that the new cross-sectional area A_f (i.e., the area normal to the uniaxial fiber force) is simply $A\cos\gamma = JA_o|\underset{\sim}{\mathbf{n}}|\cos\gamma$, where γ is the angle between $\underset{\sim}{\mathbf{m}}$ and $\underset{\sim}{\mathbf{n}}$. Hence, $\cos\gamma = (\underset{\sim}{\mathbf{m}} \bullet \underset{\sim}{\mathbf{n}})/(|\underset{\sim}{\mathbf{m}}||\underset{\sim}{\mathbf{n}}|)$. Noting that $\underset{\sim}{\mathbf{m}} \bullet \underset{\sim}{\mathbf{n}} = 1$ and recalling that $|\underset{\sim}{\mathbf{m}}| = \lambda$, we find that $A_f = JA_o/\lambda$.

The Cauchy stress $\underset{\approx}{\sigma}$ must be uniaxial in the fiber direction. The force per fiber is $F(\lambda)$. The number of fibers is $\nu_o A_o$. Thus, the uniaxial stress is the total force $F(\lambda)\nu_o A_o$ divided by the area *currently normal to the fiber direction*, JA_o/λ. Recalling that the magnitude of $\underset{\sim}{\mathbf{m}}$ is λ, the *exact* solution (valid for *any* deformation $\underset{\approx}{\mathbf{F}}$) for the Cauchy stress tensor $\underset{\approx}{\sigma}$ is

$$\sigma_{ij} = \frac{G(\lambda)}{J} m_i m_j \quad , \quad where \quad G(\lambda) = \nu_o \frac{F(\lambda)}{\lambda} \quad . \tag{16}$$

Hence, the exact solution for the unrotated Cauchy stress is

$$\boxed{\bar{\sigma}_{ij} = \frac{G(\lambda)}{J} \overline{m}_i \overline{m}_j} \quad where \quad \overline{m}_i = R^T_{ip} m_p = \overline{V}_{ij} \overline{M}_j \quad . \tag{17}$$

Substituting Eq. (17) into Eq. (9) shows that the *exact* solution for the PK2 stress is

$$\boxed{\bar{s}_{ij} = G(\lambda) \overline{M}_i \overline{M}_j} \quad . \tag{18}$$

These exact solutions demonstrate that the stress is a nonlinear function of strain even if the fiber force function $F(\lambda)$ is linear (affine). In other words, nonlinearity of large-distortion material response can arise as much from kinematics as from inherent material nonlinearities. An implicit goal of stress and strain measures is to (approximately) capture these kinematic contributions.

3 Exact tangent modulus tensors.

We now verify that each exact stress *rate* can be written as a fourth-order “tangent modulus” operating on the respective conjugate strain rate, as is generally assumed *a priori* in the literature. The PK2 tangent modulus (i.e., the modulus associated with the PK2 stress) possesses many of the properties usually assumed about modulus tensors. However, we will show that the Cauchy tangent modulus strongly depends on the deformation and is not even major-symmetric.

Differentiating Eq. (14), the material time rate of the fiber stretch is

$$\dot{\lambda} = \frac{\overline{M}_i \overline{M}_j \dot{\bar{\varepsilon}}_{ij}}{\lambda} = \frac{\overline{m}_i \overline{m}_j \overline{D}_{ij}}{\lambda} . \tag{19}$$

The rate of the Jacobian is

$$\dot{J} = J \delta_{kl} \overline{D}_{kl} . \tag{20}$$

Differentiating Eq. (18) using Eq. (19) shows that

$$\boxed{\dot{\bar{s}}_{ij} = \overline{E}_{ijkl} \dot{\bar{\varepsilon}}_{kl}} , \quad \textit{where} \quad \overline{E}_{ijkl} = \frac{G'(\lambda)}{\lambda} \overline{M}_i \overline{M}_j \overline{M}_k \overline{M}_l . \tag{21}$$

For small distortions (where $\overline{\mathbf{V}} \approx \mathbf{I}$), the PK2 tangent modulus tensor is

$$\overline{E}^0_{ijkl} = \nu_o F'(1) \overline{M}_i \overline{M}_j \overline{M}_k \overline{M}_l \qquad \leftarrow \quad \textit{valid for } \lambda \approx 1. \tag{22}$$

Referring to Eq. (21), the exact large-distortion PK2 tangent modulus $\overline{\mathbf{E}}$ is not generally equal to the small-distortion PK2 modulus $\overline{\mathbf{E}}^0$ except for the highly nonphysical case that $F(\lambda)$ is proportional to $\lambda(\lambda^2-1)$. Since this function has a zero slope at $\lambda = 1/\sqrt{3}$, *cavalierly using a constant PK2 modulus could lead to compression instabilities in numerical calculations*. On the other hand, the small distortion PK2 modulus does possess an appealing feature of being in the same *direction* as the exact large-distortion modulus. Such is not true for the unrotated Cauchy stress, as shown below.

Deriving an *exact* solution for the Cauchy stress rate is straightforward but moderately complicated and, as it happens, not necessary. The quantities λ, J and $\overline{\mathbf{m}}$ are all functions of $\overline{\mathbf{V}}$. Consequently, their rates are all linear in $\dot{\overline{\mathbf{V}}}$. Equation (12) may be solved to give $\dot{\overline{\mathbf{V}}}$ as a linear function of $\overline{\mathbf{D}}$ (invertibility follows by considering the equation in the principal basis of $\overline{\mathbf{V}}$). Thus the chain rule may be applied to Eq. (17) to show that the *exact* rate of the unrotated Cauchy stress is linear in $\overline{\mathbf{D}}$, i.e., there *does* exist a (complicated) fourth-order Cauchy tangent tensor $\overline{\mathbf{L}}$ — which is a function of the stretch $\overline{\mathbf{V}}$, but is independent of $\overline{\mathbf{D}}$ — such that the exact solution for the unrotated Cauchy stress may be written

$$\boxed{\dot{\bar{\sigma}}_{ij} = \overline{L}_{ijkl} \overline{D}_{kl}} . \tag{23}$$

The existence of a Cauchy tangent tensor $\bar{\mathbf{L}}$ is often presumed in the literature, and this result validates such an assumption for our fiber material, However, its complicated dependence on the state of deformation adulterates its usual interpretation as a material property. Furthermore, another common assumption about the *nature* of $\bar{\mathbf{L}}$ (namely, that it is major-symmetric) is generally inappropriate, as discussed in Section 4.

We now examine the structure of the tensor $\bar{L}_{ijkl}$ in more detail. The exact solution, Eq. (17), for the unrotated Cauchy stress may be written

$$\bar{\sigma}_{ij} = h\,\bar{p}_i \bar{p}_j, \tag{24}$$

where

$$\bar{\mathbf{p}} \equiv \frac{\bar{\mathbf{m}}}{\sqrt{\bar{\mathbf{m}} \bullet \bar{\mathbf{m}}}} = \frac{\bar{\mathbf{m}}}{\lambda} \qquad \textit{and} \qquad h \equiv \frac{\lambda^2 G(\lambda)}{J}. \tag{25}$$

Here, $\bar{\mathbf{p}}$ is simply a unit vector in the direction of $\bar{\mathbf{m}}$ and h is a scalar function of the stretch λ and the Jacobian J (also note that h=0 if and only if λ=1). Recalling Eqs. (19) and (20),

$$\dot{h} = (\eta\, \bar{p}_k \bar{p}_l - h\, \delta_{kl}) \bar{D}_{kl} \qquad \textit{where} \qquad \eta \equiv \frac{\lambda^2}{J}[2G(\lambda) + \lambda G'(\lambda)]\ . \tag{26}$$

Hence, the exact solution for the rate of the unrotated Cauchy stress is of the form

$$\dot{\bar{\sigma}}_{ij} = \bar{p}_i \bar{p}_j (\eta\, \bar{p}_k \bar{p}_l - h\, \delta_{kl}) \bar{D}_{kl} + h(\dot{\bar{p}}_i \bar{p}_j + \bar{p}_i \dot{\bar{p}}_j)\ . \tag{27}$$

Noting that $\dot{\bar{\mathbf{p}}}$ is always perpendicular to $\bar{\mathbf{p}}$, *the stress rate is not uniaxial* even though the stress itself *is* uniaxial.

The rate of $\bar{\mathbf{p}}$ is given by

$$\dot{\bar{p}}_i = \bar{A}_{ij} \bar{p}_j - \bar{p}_i (\bar{p}_j \bar{p}_k \bar{D}_{jk}), \quad \textit{where} \quad \bar{A}_{ij} \equiv \dot{\bar{V}}_{ik} \bar{V}^{-1}_{kj} = \bar{D}_{ij} - \bar{H}_{ij}\ . \tag{28}$$

Here $\bar{\mathbf{H}} = \bar{\boldsymbol{\Omega}} - \bar{\mathbf{W}}$, where $\bar{\boldsymbol{\Omega}}$ is the unrotated spin ($= \mathbf{R}^T \bullet \dot{\mathbf{R}}$) and $\bar{\mathbf{W}}$ is the unrotated vorticity. Dienes [2] showed that $\bar{\mathbf{H}}$ can be expressed as a linear function of $\bar{\mathbf{D}}$ and, hence, so can $\bar{\mathbf{A}}$, thereby again demonstrating that the entire right-hand side of Eq. (27) may be expressed in the form of Eq. (23). However, $\bar{\mathbf{A}}$ is *equal* to $\bar{\mathbf{D}}$ if and only if $\bar{\mathbf{V}}$ and $\dot{\bar{\mathbf{V}}}$ share the same principal axes, which describes a class of “proportional stretching” deformations not uncommon in laboratory experiments and useful in subsequent examples.

Below, we confirm Zheng’s assertion [3] that the tensor $\bar{\mathbf{L}}$ in Eq. (23) must be transversely isotropic about a privileged direction parallel to $\bar{\mathbf{m}}$, not $\bar{\mathbf{M}}$. We show, however, that $\bar{\mathbf{L}}$ has an unexpected structure. Since the fibers are all parallel to $\bar{\mathbf{m}}$, and because the material has no resistance to shear along the fiber directions, it would *seem* natural to take $\bar{L}_{ijkl} = E\bar{p}_i\bar{p}_j\bar{p}_k\bar{p}_l$, where E is a material constant. If this conjecture were true, however, the unrotated stress *rate* would be proportional to $\bar{p}_i\bar{p}_j$ — that is, it would be uniaxial, in contradiction to the exact solution Eq. (27) except for small fiber stretches (so that $h\approx 0$) or for deformations that do not distort the fibers from their initial orientation (so that $\dot{\bar{\mathbf{p}}} = \mathbf{0}$).

Recall that $\bar{\mathbf{L}}$ in Eq. (23) exists for *any* deformation. We now examine the fundamental structure of $\bar{\mathbf{L}}$ for a class of deformations in which $\bar{\mathbf{V}}$ and $\dot{\bar{\mathbf{V}}}$ share the same principal axes. Then $\bar{\mathbf{A}} = \bar{\mathbf{D}}$, and Eqs. (27) and (28) combine to give

$$\dot{\bar{\sigma}}_{ij} = [-h(\delta_{kl}\bar{D}_{kl}) + (\eta - 2h)\bar{P}_{kl}\bar{D}_{kl}]\bar{P}_{ij} + h(\bar{P}_{ik}\bar{D}_{kj} + \bar{D}_{ik}\bar{P}_{kj}) \ , \qquad (29)$$

where $\bar{P}_{ij}$ is a simple projection tensor defined by

$$\bar{P}_{ij} \equiv \bar{p}_i\,\bar{p}_j \ . \qquad (30)$$

Factoring out the rate of deformation gives

$$\dot{\bar{\sigma}}_{ij} = \bar{L}^*_{ijkl}\bar{D}_{kl} - h\,(\bar{P}_{ij}\delta_{kl})\,\bar{D}_{kl} \ , \qquad (31)$$

where the Voigt-Mandel components (ordered 11, 22, 33, 23, 31, 12) of $\bar{L}^*_{ijkl}$ in terms of an orthonormal basis having the 1-direction aligned with $\bar{\mathbf{p}}$ are

$$\bar{L}^*_{ijkl} = \begin{bmatrix} \eta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h & 0 \\ 0 & 0 & 0 & 0 & 0 & h \end{bmatrix} \ . \qquad (32)$$

The tensor $\bar{\mathbf{L}}^*$ is indeed transversely isotropic about $\bar{\mathbf{p}}$, but the presence of h makes the stress *rate* have nonzero shear (23 and 31) components even though the stress itself is always uniaxial. These components arise because the fiber axis changes with material distortion, a contribution overlooked by Zheng [3]. If the distortion is severe enough that $\bar{\mathbf{m}} \neq \bar{\mathbf{M}}$, then generally $h \neq 0$ (neglecting h would be tantamount to neglecting stress itself). Put differently, it would be inconsistent to assert that $\bar{\mathbf{L}}^*$ must be transversely isotropic about $\bar{\mathbf{p}}$ while not allowing its components to include contributions from the rate of change of $\bar{\mathbf{p}}$. It would be wrong to generalize, say, Spencer's *small-distortion* expression of stress as a transverse function of strain [4] to large deformations in the unrotated configuration. Doing so misses contributions like the last term in Eq. (27).

Recalling Eqs. (5) and (8), Eq. (29) may be easily converted to spatial form for direct comparison with Zheng's generalization of a transversely isotropic constitutive equation from its arotational form [3]. Zheng's Eq. (4.5) fails to capture the last term in Eq. (31), unless $h = 0$ (which is possible only for the uninteresting case of unstretched fibers) or $\bar{D}_{kk} = 0$ (also a very restrictive condition). Furthermore, recall there is no comparison whatsoever without the assumption that $\bar{\mathbf{V}}$ and $\dot{\bar{\mathbf{V}}}$ share the same principal axes, representing yet another restriction that would have to be placed on the deformation in order to obtain good results using Zheng's expression. It might appear at first glance that the last term in Zheng's Eq. (4.5) captures at least the qualitative character of the last term in Eq. (29), but Zheng's term arises *not* from the rate of rotation of the fibers, but simply from the shear resistance of the material, which must be zero for the idealized fiber material. As discussed in Section 5, Zheng's approach for generalizing arotational constitutive laws seems incapable of capturing certain distinctions in material response that arise from the microstructure. Of course, despite these defects, Zheng's model is far superior to any model that takes the reference transverse axis of symmetry to be unchanged by distortion.

4 Major-symmetry of tangent tensors

The fourth-order tensor $h\bar{p}_i\bar{p}_j\delta_{kl}$ in the second term of Eq. (31) is transversely isotropic about $\bar{\mathbf{p}}$, but it is *not* major-symmetric. Hence, in the exact solution (Eq. 23), the tensor $\bar{\mathbf{L}}$ is not major-symmetric (i.e., $\bar{L}_{ijkl} \neq \bar{L}_{klij}$). The existence of an elastic energy function is often used to justify an assumption of major-symmetry. The argument is subtle for large deformations where, in the absence of thermal power,[1] the first law of thermodynamics requires that

$$\rho \dot{e} = \sigma_{ij} D_{ij} = \bar{\sigma}_{ij} \bar{D}_{ij} \quad . \tag{33}$$

Here, ρ is the density and e is the internal energy per unit mass. Note that $\bar{\sigma}_{ij} \bar{D}_{ij}$ is *not* the true rate of any path-independent quantity, while $(\bar{\sigma}_{ij}/\rho)\bar{D}_{ij}$ *is* a true rate. Equivalently, $(J\bar{\sigma}_{ij})\bar{D}_{ij}$ is a true rate. The non-major-symmetric term in Eq. (31) would not be present if we had instead differentiated the exact solution for $J\bar{\sigma}_{ij}$. This is, in fact, a general result as shown below.

In terms of the PK2 stress $\bar{\mathbf{s}}$ and Lagrange strain $\bar{\varepsilon}$, the first law of thermodynamics (without thermal power) is

$$\rho_o \dot{e} = \bar{s}_{ij} \dot{\bar{\varepsilon}}_{ij} \quad , \tag{34}$$

For a closed elastic system, the PK2 stress is taken to be a (material) function of strain, and it follows from Eq. (34) that this function is derivable from a potential (the energy):

$$\frac{\bar{s}_{ij}}{\rho_o} = \frac{\partial e}{\partial \bar{\varepsilon}_{ij}} \quad . \tag{35}$$

Hence, applying the chain rule noting that the material rate of ρ_o is zero,

$$\dot{\bar{s}}_{ij} = \bar{E}_{ijkl} \dot{\bar{\varepsilon}}_{kl} \ , \qquad where \qquad \bar{E}_{ijkl} = \rho_o \left[\frac{\partial^2 e}{\partial \bar{\varepsilon}_{ij} \partial \bar{\varepsilon}_{kl}} \right] . \tag{36}$$

As long as the energy e is sufficiently differentiable, the fourth-order tensor $\bar{\mathbf{E}}$ possesses major symmetry.

A similar analysis cannot be performed directly on Eq. (33) because $\bar{\mathbf{D}}$ is not a true rate with respect to deformation.[2] Instead, Eq. (36) must be rephrased in terms of Cauchy stress.

Recalling that $J = \rho_o / \rho$, Eq. (9) may be written

$$\frac{\bar{\sigma}_{ij}}{\rho} \equiv \bar{V}_{ip} \bar{V}_{jq} \frac{\bar{s}_{pq}}{\rho_o} \quad . \tag{37}$$

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[1]Including thermal power would not change our ultimate conclusions.

[2]There does not generally exist a tensor ξ that depends only on the deformation $\mathbf{F}$ such that $\bar{\mathbf{D}} = \dot{\xi}$.

Differentiating this expression using Eqs. (36), (12), and (10) shows that the material rate of the specific stress is

$$\frac{D}{Dt}\left(\frac{\bar{\sigma}_{ij}}{\rho}\right) = \left(\bar{V}_{ip}\bar{V}_{jq}\bar{V}_{kr}\bar{V}_{ls}\frac{\bar{E}_{pqrs}}{\rho J}\right)\bar{D}_{kl} + \dot{\bar{V}}_{ip}\bar{V}^{-1}_{pq}\frac{\bar{\sigma}_{qj}}{\rho} + \frac{\bar{\sigma}_{ip}}{\rho}\bar{V}^{-1}_{pq}\dot{\bar{V}}_{qj} \quad . \tag{38}$$

Recalling that $\dot{\bar{\mathbf{V}}}$ is linear in $\bar{\mathbf{D}}$, this result proves that for *any* deformation path there *does exist* a fourth-order tensor $\bar{\mathbf{C}}$ such that

$$\frac{D}{Dt}\left(\frac{\bar{\sigma}_{ij}}{\rho}\right) = \frac{1}{\rho}\bar{C}_{ijkl}\bar{D}_{kl} \quad . \tag{39}$$

Noting that $\dot{\rho} = -\rho\delta_{ij}\bar{D}_{ij}$, this result also confirms the existence of a Cauchy tangent tensor $\bar{\mathbf{L}}$ such that $\dot{\bar{\sigma}}_{ij} = \bar{L}_{ijkl}\bar{D}_{kl}$. To demonstrate the claim that $\bar{\mathbf{L}}$ is not necessarily major symmetric, it is sufficient to consider proportional stretching paths where $\bar{\mathbf{V}}$ and $\dot{\bar{\mathbf{V}}}$ share principal axes. Then recalling the discussion following Eq. (28), Eq. (38) becomes

$$\bar{C}_{ijkl} = \frac{1}{J}\bar{V}_{ip}\bar{V}_{jq}\bar{V}_{kr}\bar{V}_{ls}\bar{E}_{pqrs} + \frac{1}{2}(\delta_{ik}\bar{\sigma}_{jl} + \delta_{jl}\bar{\sigma}_{ik} + \delta_{il}\bar{\sigma}_{jk} + \delta_{jk}\bar{\sigma}_{il}) . \tag{40}$$

Since $\bar{\mathbf{E}}$ possesses major symmetry, so does $\bar{\mathbf{C}}$. Noting that $\dot{\rho} = -\rho\delta_{ij}\bar{D}_{ij}$, Eq. (39) may be written $\dot{\bar{\sigma}}_{ij} = \bar{L}_{ijkl}\bar{D}_{kl}$, where

$$\bar{L}_{ijkl} = \bar{C}_{ijkl} - \bar{\sigma}_{ij}\delta_{kl} \quad , \tag{41}$$

which is *not* major symmetric. This example of proportional stretching proves that the rate of stress *itself* is not generally expressible as a *major-symmetric* tensor operating on $\bar{\mathbf{D}}$ because volumetric contributions [second term in Eq. (41), or second term in Eq. (31)] are not major-symmetric. Bergander [5] mentions that Kirchhoff's stress tensor $J\boldsymbol{\sigma}$ is routinely used in modern constitutive models, though sometimes without any justification other than convenience. The above discussion shows that using specific stress (or Kirchhoff's stress tensor, $J\boldsymbol{\sigma}$) endows a major symmetry to the conjugate tangent modulus tensor, which is an appealing and useful property for many applications. *However*, the fiber example studied earlier shows that even if Kirchhoff's stress is used, the associated tangent modulus tensor cannot sensibly be regarded as a material property — it must change as the material distorts.

5 Microstructure affects macrostructure

We now mention that the Cauchy tangent tensor must “distort with the material” in a way that depends on the microstructure. In Fig. 2, a fiber composite and a laminate are each subjected to the same *macroscopic* pure stretch. Both composites are initially transversely isotropic with the same axis of symmetry ($\bar{\mathbf{M}} = \bar{\mathbf{N}}$). Upon distortion, the symmetry axis moves *with the material* in the fiber case, but with the material *planes* in the laminate case. For the fiber case, Zheng [3] correctly pointed out that a large deformation law of the form $\dot{\sigma} = f(\bar{\mathbf{D}})$ must also depend on the *distorted* fiber direction $\bar{\mathbf{m}} = \bar{\mathbf{V}} \bullet \bar{\mathbf{M}}$, not the reference direction $\bar{\mathbf{M}}$. We have already shown [Eq. (27)] that *it must additionally depend on the rate* $\dot{\bar{\mathbf{m}}}$. In the laminate case, the function *f* apparently must depend on the distorted laminate plane *normal* $\bar{\mathbf{n}}$ (and its rate). To accommodate these microstructural considerations, a numerical model (e.g., [6]) might require the user to specify whether the material possesses a fiber or a laminate microstructure, though such an approach might be stymied by “exotic” laminates whose layers are fiber composites. Zheng did not discuss the alternative law of the form $\dot{\mathbf{s}} = g(\dot{\varepsilon})$, where the PK2 function *g* apparently depends on the *undistorted* reference direction in both the fiber and laminate cases, again suggesting that the PK2 description might be better suited for large-distortion analyses of anisotropic materials.

6 Conclusions

This paper has reviewed several important caveats regarding large-distortion constitutive laws. Namely, *a sensible large-distortion constitutive law generally cannot be constructed from a small-distortion law by simply applying the small-distortion law in the unrotated configuration, even though frame indifference is satisfied*. Any anisotropic constitutive law phrased in terms of unrotated Cauchy stress $\bar{\underset{\sim}{\sigma}}$ and rate-of-deformation $\bar{\underset{\approx}{\mathbf{D}}}$ must account for distorted material directions. For our fiber example, this means that the Cauchy tangent stiffness tensor must depend *not* on the initial fiber orientation $\bar{\underset{\sim}{\mathbf{M}}}$, but on the distorted orientation $\bar{\mathbf{m}}$, *and its rate* $\dot{\bar{\mathbf{m}}}$. Furthermore, *the Cauchy stress $\underset{\sim}{\sigma}$ must be replaced by the specific stress $\underset{\sim}{\sigma}/\rho$ or Kirchhoff's stress $J\underset{\sim}{\sigma}$ if the associated tangent modulus tensor is to possess major symmetry for general deformations*. Comparing a fiber composite with a laminate composite having the same transverse axis of symmetry demonstrates that *the microstructural source of the anisotropy must be explicitly accommodated for any large-distortion problem modeled using unrotated Cauchy stress with the unrotated rate-of-deformation*. These complications associated with distortions of the material directions can be managed by using the second Piola-Kirchhoff stress of Eq. (9) together with the Lagrange strain of Eq. (11). For this conjugate pair, the tangent modulus possesses major symmetry and depends on the initial (not distorted) material directions; hence, there are no counterintuitive contributions from material direction rates. However, to avoid numerical instabilities, *the PK2 modulus magnitude must still be determined by high-distortion experiments*.

Acknowledgments

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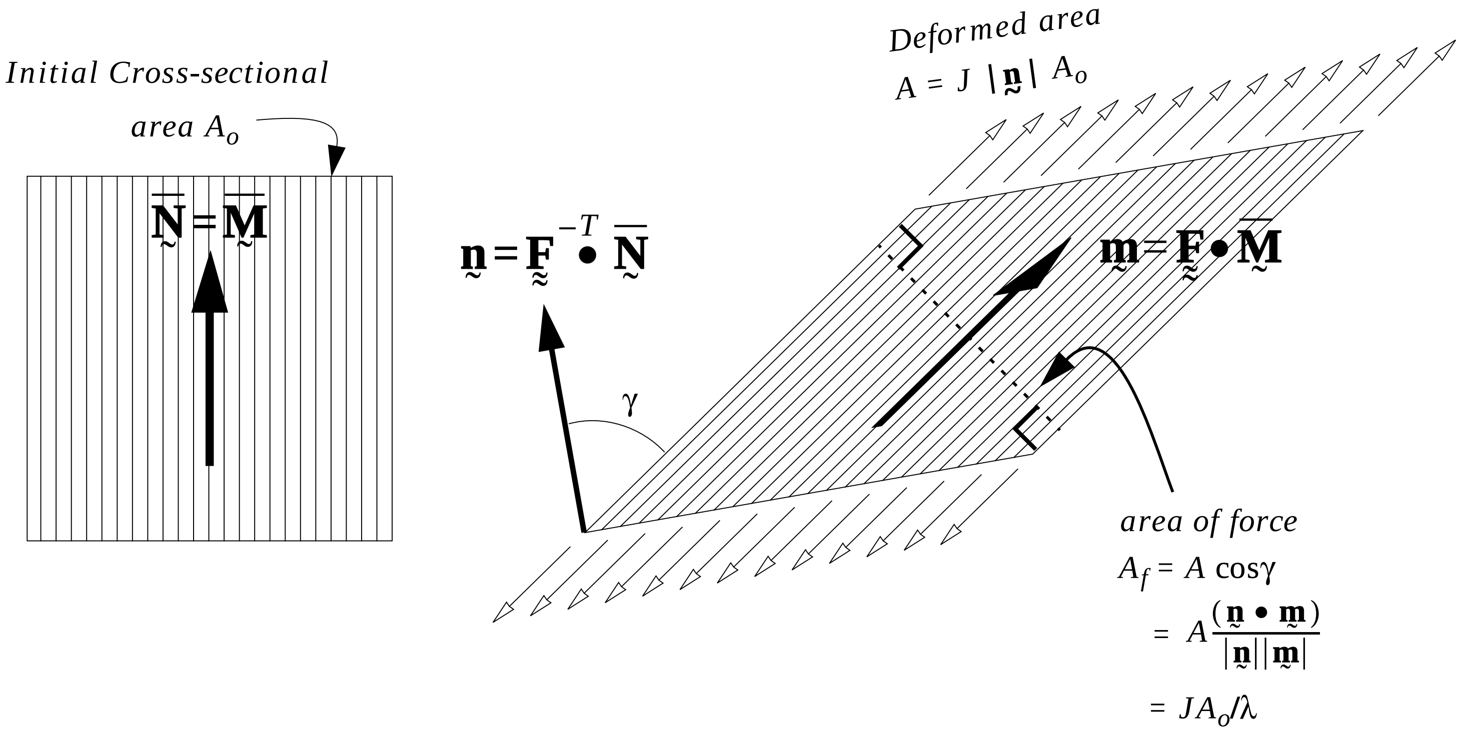

Fig. 1. An idealized array of fibers in a negligibly stiff matrix (e.g., air). The fibers distort to a new orientation parallel to $\underset{\sim}{m}$ (the magnitude of which is the fiber stretch λ). The cross-sectional area A_o originally normal to the fiber direction distorts to a new orientation parallel to $\underset{\sim}{n}$ (not a unit vector). The right side of the figure shows the distorted shape as seen in the plane spanned by $\underset{\sim}{n}$ and $\underset{\sim}{m}$.

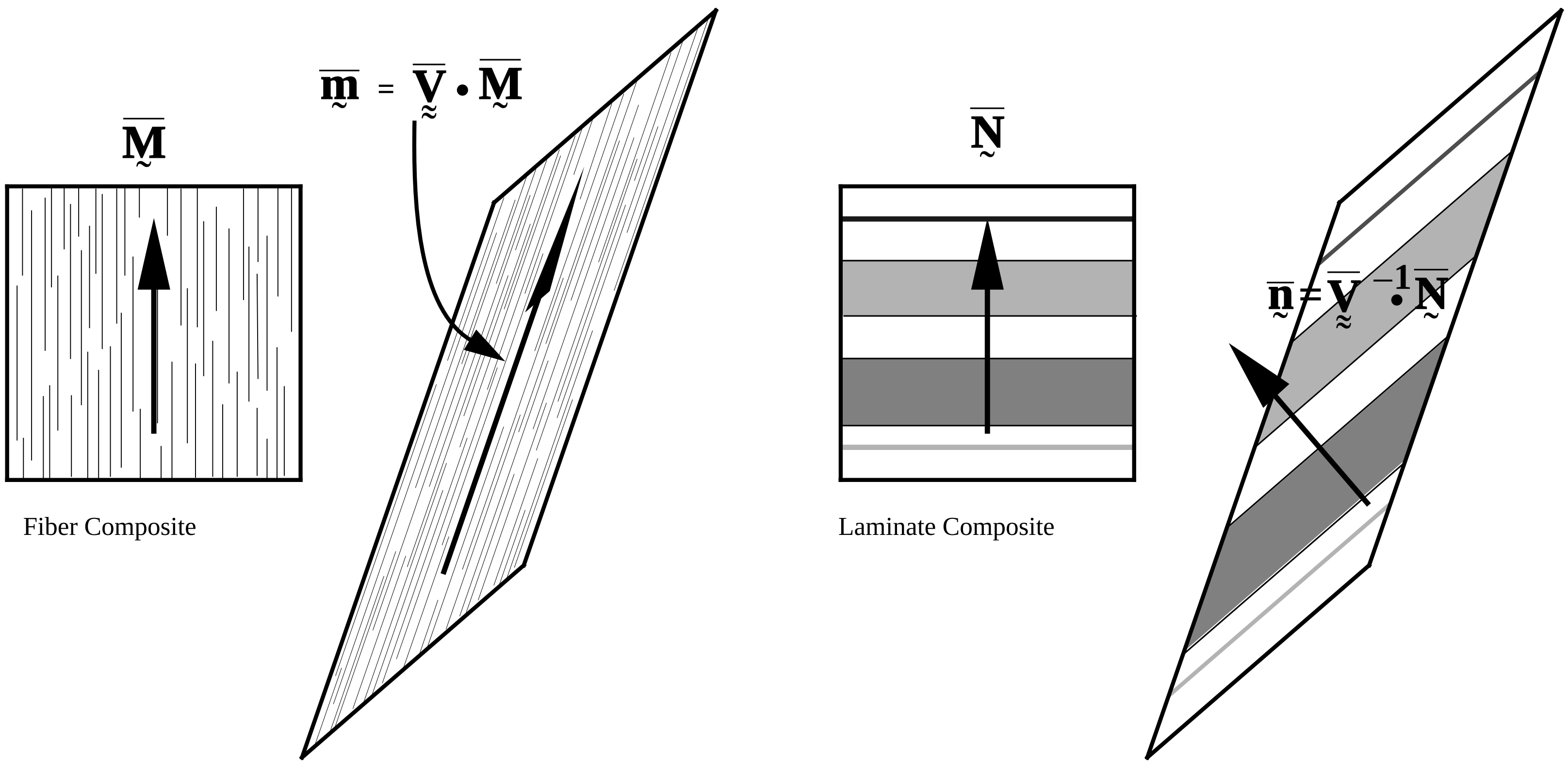

Fig. 2. Two initially transversely isotropic microstructures suffering pure shear with enough superimposed rotation to make $\underset{\sim}{\mathbf{R}}=\underset{\sim}{\mathbf{I}}$. The macroscopic symmetry axes move in a way that depends on the microscopic source of the anisotropy.