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Abstract

In their original formulation of the method of isotropic extension via structural tensors, which is meant for applications to the derivation of coordinate-free representation formulas for anisotropic constitutive functions, both Boehler and Liu start with the assumption that the invariance group of structural tensors is the symmetry group that defines the anisotropy of the constitutive function in question. As a result, the method (with structural tensors of order not higher than two) is applicable only when the anisotropy is characterized by a cylindrical group or belongs to the triclinic, monoclinic, or rhombic crystal classes. In this note we present a reformulation of the method in which the aforementioned assumption of Boehler and of Liu is relaxed, and we show by examples in finite elasticity and anisotropic linear elasticity that the method of isotropic extension via structural tensors could be applicable beyond the original limitations.

Keywords

Anisotropic constitutive functions, isotropic extension, structural tensors

I. Method of isotropic extension as formulated by Boehler and by Liu

General representation theorems have long been obtained [1-3] for isotropic scalar-, vector-, and second-order tensor-valued functions of a finite number of vectors and second-order tensors. To make use of these general theorems, Boehler [4] and Liu [5] independently proposed the same method to derive coordinatefree representation formulas for anisotropic constitutive functions. Take Liu [5] for definiteness. There he begins with the observation that "[m]any anisotropic materials possess structures which can be characterized by certain directions, lines or planes, more specifically, say characterized by some unit vectors" $m_1, ..., m_r$, "and some [second-order] tensors" $M_1, ..., M_s$. For brevity, we henceforth put

$$\vec{m} := (m_1, ..., m_r), \qquad \vec{M} := (M_1, ..., M_s),$$
(1)

and refer to m_k (k = 1, ..., r) and M_l (l = 1, ..., s) as the structural tensors, which are specific first- and secondorder tensors that characterize the anisotropic material response in question. Let O(3) denote the group of



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orthogonal transformations on V, the translation space of the three-dimensional physical space. For $Q \in O(3)$ let

$$\boldsymbol{Q}\boldsymbol{\vec{m}} := (\boldsymbol{Q}\boldsymbol{m}_1, ..., \boldsymbol{Q}\boldsymbol{m}_r), \qquad \boldsymbol{Q}\boldsymbol{\vec{M}}\boldsymbol{Q}^{\mathrm{T}} := (\boldsymbol{Q}\boldsymbol{M}_1\boldsymbol{Q}^{\mathrm{T}}, ..., \boldsymbol{Q}\boldsymbol{M}_s\boldsymbol{Q}^{\mathrm{T}}).$$
(2)

Liu [5] introduces the group \mathcal{G}_s of orthogonal transformations that preserves each of the structural tensors, i.e.¹

$$\mathcal{G}_s := \{ \boldsymbol{Q} \in \mathcal{O}(3) : \boldsymbol{Q} \overrightarrow{\boldsymbol{m}} = \overrightarrow{\boldsymbol{m}}, \boldsymbol{Q} \overrightarrow{\boldsymbol{M}} \boldsymbol{Q}^{\mathrm{T}} = \overrightarrow{\boldsymbol{M}} \}.$$
(3)

The definition given by equation (3) is essentially the same as that given earlier by Boehler [4], who later calls \mathcal{G}_s the invariance group of the structural tensors \vec{m}, \vec{M} [6].

Let $\vec{v} = (v_1, ..., v_p)$ and $\vec{A} = (A_1, ..., A_q)$, where v_i (i = 1, ..., p) are vectors and A_j (j = 1, ..., q) are second-order tensors. Consider a class \mathcal{A} of second-order-tensor-valued anisotropic constitutive functions $S(\vec{v}, \vec{A})$ with the anisotropy characterized by a group \mathcal{G}_s of the type given by equation (3), i.e. S satisfies

$$\boldsymbol{QS}(\vec{\boldsymbol{v}},\vec{\boldsymbol{A}})\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{S}(\boldsymbol{Q}\vec{\boldsymbol{v}},\boldsymbol{Q}\vec{\boldsymbol{A}}\boldsymbol{Q}^{\mathrm{T}}) \qquad \text{for each } \boldsymbol{Q} \in \mathcal{G}_{s}. \tag{4}$$

The method that Boehler [4] and Liu [5] proposed to obtain a coordinate-free representation formula for the class \mathcal{A} of anisotropic constitutive functions S is to seek a corresponding class Ext of constitutive functions $\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$ such that for each $S \in \mathcal{A}$, there is an $\hat{S} \in \text{Ext}$ which satisfies

$$S(\vec{v}, \vec{A}) = \hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$$
(5)

for each (\vec{v}, \vec{A}) in the domain of **S** and observes the requirement² that

$$\boldsymbol{Q}\hat{\boldsymbol{S}}(\vec{v},\vec{A},\vec{m},\vec{M})\boldsymbol{Q}^{\mathrm{T}} = \hat{\boldsymbol{S}}(\boldsymbol{Q}\vec{v},\boldsymbol{Q}\vec{A}\boldsymbol{Q}^{\mathrm{T}},\boldsymbol{Q}\vec{m},\boldsymbol{Q}\vec{M}\boldsymbol{Q}^{\mathrm{T}}) \qquad \text{for each } \boldsymbol{Q} \in \mathrm{O}(3), \tag{6}$$

i.e. that \hat{S} is isotropic. Then we may appeal to representation theorems for isotropic functions to obtain a representation formula for \hat{S} and, *a fortiori*, for the anisotropic *S*. Moreover, it follows immediately from equations (3), (5) and (6) that for each $Q \in \mathcal{G}_s$

$$QS(\vec{v}, \vec{A})Q^{\mathrm{T}} = Q\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})Q^{\mathrm{T}}$$

= $\hat{S}(Q\vec{v}, Q\vec{A}Q^{\mathrm{T}}, Q\vec{m}, Q\vec{M}Q^{\mathrm{T}})$
= $\hat{S}(Q\vec{v}, Q\vec{A}Q^{\mathrm{T}}, \vec{m}, \vec{M})$
= $S(Q\vec{v}, Q\vec{A}Q^{\mathrm{T}}),$ (7)

i.e. the constitutive function S, as given by equation (5), satisfies equation (4). Conversely, Liu [5] proves (see Theorem 3.1 there) that for each anisotropic $S(\vec{v}, \vec{A})$ with anisotropy defined by an invariance group \mathcal{G}_s of structural tensors (see equation (3)), there exists an isotropic extension function $\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$ such that equation (5) holds. Liu's theorem renders Boehler's physical justification on the isotropy of \hat{S} unnecessary when $\mathcal{G} = \mathcal{G}_s$. All that we have said about anisotropic second-order-tensor-valued functions $S(\vec{v}, \vec{A})$ applies (with obvious minor modifications) also to scalar- and vector-valued functions $\psi(\vec{v}, \vec{A})$ and $u(\vec{v}, \vec{A})$. What we have outlined above is the method of isotropic extension of anisotropic constitution functions via structural tensors as formulated by Boehler and by Liu.

As the method of Boehler and Liu treats only material symmetries characterized by invariance groups of structural tensors, a question naturally arises, namely: Which subgroups of O(3) can be taken as an invariance group of structural tensors of order not higher than two? For the special case where the anisotropic S maps a finite number of second-order symmetric tensors to second-order symmetric tensors, Boehler [4] asserts that besides transverse isotropy "the method proposed covers also all the crystal classes of the triclinic, monoclinic and rhombic systems." He does not say anything about the other crystal classes in his paper. Liu [5] remarks that "[0]bviously, not every anisotropic material can be specified by symmetry group of the type" given by equation (3), but he does not elaborate on what to him is obvious. Later in the same paper he gives a list ("which does not mean to be exhaustive") of groups $\mathcal{G}_s \subset O(3)$ that are characterized by some set $\{\vec{m}, \vec{M}\}$ of structural tensors

in the sense specified by equation (3). Besides transverse isotropy and orthotropy, Liu's list includes groups pertaining to crystal classes in the triclinic, monoclinic, and rhombic systems. More recently, Xiao et al. [9] demonstrated that "any number of vectors and second order tensors can merely characterize and represent one of the cylindrical groups and the triclinic, monoclinic, rhombic crystal classes." They proceed to assert what follows:

This suggests that, for anisotropic functions relative to any anisotropic material symmetry group other than those just mentioned, the widely used isotropic extension method via structural tensors has to result in isotropic extension functions involving at least one structural tensor variable of order higher than two.

But as Xiao et al. point out, "partial results for a simple case ... already suggest as examples formidable complexity" of "unconventional isotropic functions involving at least one tensor variable of order higher than two".

We contend that the aforementioned limitations of the method of isotropic extension via structural tensors (of order not higher than two) arise from an unnecessary requirement in the original formulation of both Boehler and Liu, namely that the material symmetry in question be characterized by a group which keeps each structural tensor invariant. After a reformulation which relaxes this requirement, it will become possible that the method of isotropic extension could cover anisotropic constitutive functions with anisotropy defined by a symmetry group which cannot be taken as an invariance group of structural tensors of order not higher than two. Before we proceed further, we present some simple examples in finite and linear elasticity that will suggest how the reformulation should be made.

2. Simple examples in finite and linear elasticity

2.1. Finite elasticity

Consider an elastic material point with a chosen undistorted reference configuration. Let F be the deformation gradient, F = RU the polar decomposition of F, where R is the rotation tensor and U the right stretch tensor, and $C := U^2$ the right Cauchy-Green tensor. Let T be the Cauchy stress. The elastic response of the material point is given by the constitutive function T = T(F). The principle of material frame-indifference dictates that

$$T(F) = R\overline{T}(C)R^{\mathrm{T}}$$
(8)

for some function $\overline{T}(C)$. Conversely for any function $\overline{T}(C)$, the function T(F) given by equation (8) satisfies material frame-indifference. Let

$$\mathcal{G} := \{ \mathbf{P} \in \mathcal{O}(3) : \mathbf{T}(\mathbf{FP}) = \mathbf{T}(\mathbf{F}) \text{ for each } \mathbf{F} \text{ in the domain of } \mathbf{T}(\cdot) \}$$

be the symmetry group of the elastic material point in question. The function $\overline{T}(C)$ in equation (8) satisfies

$$\boldsymbol{Q}\overline{\boldsymbol{T}}(\boldsymbol{C})\boldsymbol{Q}^{\mathrm{T}} = \overline{\boldsymbol{T}}(\boldsymbol{Q}\boldsymbol{C}\boldsymbol{Q}^{\mathrm{T}}) \qquad \text{for each } \boldsymbol{Q} \in \mathcal{G}.$$
⁽⁹⁾

Note that equation (9) is the specific form assumed by equation (4) in the present context. For details on these preliminaries see, e.g. Truesdell [7].

If $\overline{T}(C)$ has an isotropic extension $\hat{T}(C, \overline{m}, \overline{M})$, substitution of \hat{T} for \overline{T} in equation (8) yields

$$T(F) = R\dot{T}(C, \vec{m}, \vec{M})R^{\mathrm{T}}$$

= $\hat{T}(B, R\vec{m}, R\vec{M}R^{\mathrm{T}}),$ (10)

where $B = RCR^{T}$ is the left Cauchy-Green tensor. Consideration of material frame-indifference suggests that structural tensors in $\{\vec{m}, \vec{M}\}$, like *C*, remain unchanged under change of frame, and they pertain to the reference configuration. It follows that members of $\{R\vec{m}, R\vec{M}R^{T}\}$, like *B*, are defined on the current configuration and they are objective. Moreover, the isotropy of the constitutive function $\hat{T}(B, R\vec{m}, R\vec{M}R^{T})$ implies that it satisfies material frame-indifference.

Conversely, one may start by postulating

$$T = \hat{T}(B, R\vec{m}, R\vec{M}R^{\mathrm{T}})$$
(11)

as the current-configuration form of the constitutive function of the elastic material point. The principle of material frame-indifference dictates that the function \hat{T} in equation (11) should satisfy the version of equation (6) for the present context, i.e. that \hat{T} be isotropic. In fact, this approach will make anisotropic finite elasticity fit into the theoretical scheme outlined by Boehler [4].

Now, let e_i (i = 1, 2, 3) be a right-handed orthonormal triad of vectors in V. Let $\mathbf{R}(n, \omega)$ denote the rotation of angle ω about the axis defined by unit vector n. Suppose the elastic material point in question is orthotropic, and its symmetry group is $\mathcal{G} = D_{2h}$ with generators $\mathbf{R}(e_2, \pi)$, $\mathbf{R}(e_3, \pi)$, and the inversion -I, where I is the second-order identity tensor. We want to seek an isotropic extension of the function $\overline{T}(C)$ for this orthotropic material.

Let $M_1 := e_1 \otimes e_1$, $M_2 := e_2 \otimes e_2$, and $M_3 := e_3 \otimes e_3$. Clearly $QM_iQ^T = M_i$ (i = 1, 2, 3) for each $Q \in \mathcal{G}$, and \mathcal{G} is the subgroup of O(3) that keeps each M_i invariant, i.e. \mathcal{G} is the invariance group \mathcal{G}_s of the structural tensors M_1, M_2 , and M_3 . Using M_i (i = 1, 2, 3) as structural tensors, Boehler [8] applies representation theorems for isotropic functions to write down an isotropic extension for orthotropic functions that map second-order symmetric tensors. As applied to $\overline{T}(C)$, the formula reads

$$T(C) = T(C, M_1, M_2, M_3)$$

:= $\alpha_1 M_1 + \alpha_2 M_2 + \alpha_3 M_3 + \alpha_4 (M_1 C + C M_1)$
+ $\alpha_5 (M_2 C + C M_2) + \alpha_6 (M_3 C + C M_3) + \alpha_7 C^2$, (12)

where

$$\alpha_i = \alpha_i (\operatorname{tr} M_1 C, \operatorname{tr} M_2 C, \operatorname{tr} M_3 C, \operatorname{tr} M_1 C^2, \operatorname{tr} M_2 C^2, \operatorname{tr} M_3 C^2, \operatorname{tr} C^3)$$

= $\tilde{\alpha}_i (C, M_1, M_2, M_3)$ (13)

for i = 1, ..., 7. Since $\mathcal{G} = \mathcal{G}_s$, by Liu's theorem [5] every $\overline{T}(C)$ has an isotropic extension $\hat{T}(C, M_1, M_2, M_3)$ given by the representation formula (12).

Now suppose the elastic material point in question is tetragonal, and its symmetry group is $\mathcal{G} = D_{4h}$ with generators $\mathbf{R}(\mathbf{e}_2, \pi)$, $\mathbf{R}(\mathbf{e}_3, \pi/2)$, and $-\mathbf{I}$. Since

$$\mathbf{R}(\mathbf{e}_3, \pi/2) \mathbf{M}_1 \mathbf{R}(\mathbf{e}_3, \pi/2)^{\mathrm{T}} = \mathbf{M}_2, \qquad \mathbf{R}(\mathbf{e}_3, \pi/2) \mathbf{M}_2 \mathbf{R}(\mathbf{e}_3, \pi/2)^{\mathrm{T}} = \mathbf{M}_1,$$

the symmetry group \mathcal{G} of the tetragonal material is not an invariance group of the structural tensors M_i (i = 1, 2, 3). On the other hand, note that each $Q \in \mathcal{G}$ either keeps all M_i invariant or keeps M_3 invariant and permutes M_1, M_2 .

In the representation formula (12), let us impose additional conditions on the coefficient $\tilde{\alpha}_i$ such that

$$\tilde{\alpha}_1(\boldsymbol{C}, \boldsymbol{M}_1, \boldsymbol{M}_2, \boldsymbol{M}_3) = \tilde{\alpha}_2(\boldsymbol{C}, \boldsymbol{M}_2, \boldsymbol{M}_1, \boldsymbol{M}_3), \quad \tilde{\alpha}_4(\boldsymbol{C}, \boldsymbol{M}_1, \boldsymbol{M}_2, \boldsymbol{M}_3) = \tilde{\alpha}_5(\boldsymbol{C}, \boldsymbol{M}_2, \boldsymbol{M}_1, \boldsymbol{M}_3),$$

$$\tilde{\alpha}_3, \tilde{\alpha}_6, \tilde{\alpha}_7 \text{ are symmetric in } \boldsymbol{M}_1 \text{ and } \boldsymbol{M}_2.$$
(14)

Then the isotropic extension \hat{T} is symmetric in M_1 and M_2 , i.e.

$$\hat{T}(C, M_1, M_2, M_3) = \hat{T}(C, M_2, M_1, M_3).$$
 (15)

It follows that under these conditions the isotropic extension (12) satisfies

$$\hat{\boldsymbol{T}}(\boldsymbol{C}, \boldsymbol{Q}\boldsymbol{M}_{1}\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}\boldsymbol{M}_{2}\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}\boldsymbol{M}_{3}\boldsymbol{Q}^{\mathrm{T}}) = \hat{\boldsymbol{T}}(\boldsymbol{C}, \boldsymbol{M}_{1}, \boldsymbol{M}_{2}, \boldsymbol{M}_{3}) \quad \text{for each } \boldsymbol{Q} \in \mathcal{G}.$$
(16)

Conversely, given a function $\overline{T}(C)$ that pertains to an elastic material point with symmetry group $\mathcal{G} = D_{4h}$ as described above, the material point is *a fortiori* orthotropic, so there exists an isotropic extension of $\overline{T}(C)$, namely $\hat{T}(C, M_1, M_2, M_3)$, which can be cast in the form of equation (12). It is easy to verify that the coefficients $\tilde{\alpha}_i$ of the isotropic extension $\hat{T}(C, M_1, M_2, M_3)$ in equation (12) must satisfy the additional conditions given by equation (14) for it to satisfy the requirement given by equation (16) for material symmetry. Hence, in the isotropic extension given by equation (12) plus the additional conditions given by equation (14) we have arrived at a representation formula for the constitutive function $\overline{T}(C)$ with tetragonal symmetry.

Similarly, if we impose on equation (12) the conditions

$$\tilde{\alpha}_{1}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{2}(C, M_{2}, M_{1}, M_{3}), \quad \tilde{\alpha}_{2}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{3}(C, M_{1}, M_{3}, M_{2}), \\
\tilde{\alpha}_{3}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{1}(C, M_{3}, M_{2}, M_{1}), \quad \tilde{\alpha}_{4}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{5}(C, M_{2}, M_{1}, M_{3}), \\
\tilde{\alpha}_{5}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{6}(C, M_{1}, M_{3}, M_{2}), \quad \tilde{\alpha}_{6}(C, M_{1}, M_{2}, M_{3}) = \tilde{\alpha}_{4}(C, M_{3}, M_{2}, M_{1}), \\
\tilde{\alpha}_{7} \text{ is symmetric in } M_{1}, M_{2}, \text{ and } M_{3},$$
(17)

the resulting representation formula gives an isotropic extension of $\overline{T}(C)$ when the symmetry group is O_h , i.e. the elastic material point has cubic symmetry.

2.2. Linear elasticity

For further illustration and for later use, here we briefly revisit the examples above in the context of linear elasticity. Let *E* be the infinitesimal strain. For the orthotropic material point with symmetry group $\mathcal{G} = \mathcal{G}_s$, the invariance group of the structural tensors $M_i = e_i \otimes e_i$ (i = 1, 2, 3), the stress-strain relation T = T(E) satisfies the equation

$$T(QEQ^{\mathrm{T}}) = QT(E)Q^{\mathrm{T}} \qquad \text{for each } Q \in \mathcal{G},$$
(18)

where $\mathcal{G} = D_{2h} = \mathcal{G}_s$ for the present case. By Liu's theorem [5], for each orthotropic T(E), an isotropic extension $\hat{T}(E, M_1, M_2, M_3)$ exists, for which Boehler [8] provides the representation formula

$$T(E) = T(E, M_1, M_2, M_3)$$

$$:= (\alpha_1 \operatorname{tr}(M_1 E) + \alpha_2 \operatorname{tr}(M_2 E) + \alpha_3 \operatorname{tr}(M_3 E))M_1$$

$$+ (\alpha_2 \operatorname{tr}(M_1 E) + \beta_2 \operatorname{tr}(M_2 E) + \beta_3 \operatorname{tr}(M_3 E))M_2$$

$$+ (\alpha_3 (\operatorname{tr}(M_1 E) + \beta_3 \operatorname{tr}(M_2 E)) + \gamma \operatorname{tr}(M_3 E))M_3$$

$$+ \alpha_4 (M_1 E + EM_1) + \alpha_5 (M_2 E + EM_2) + \alpha_6 (M_3 E + EM_3),$$
(19)

where α_k ($k = 1, 2, \dots, 6$), β_2, β_3, γ are undetermined coefficients.

Now consider the tetragonal case where $\mathcal{G} = D_{4h}$ as described in the preceding subsection. Let us impose the conditions $\beta_2 = \alpha_1$, $\beta_3 = \alpha_3$, and $\alpha_4 = \alpha_5$ on the coefficients in the representation formula (19) so that the isotropic extension \hat{T} is symmetric in M_1 and M_2 , i.e.

$$\hat{T}(E, M_1, M_2, M_3) = \hat{T}(E, M_2, M_1, M_3).$$
 (20)

Keeping the coefficients $\alpha_1, \alpha_3, \alpha_5$ and rewriting γ as α_4 , we obtain from (19) the representation formula

$$\begin{split} T(E) &= \hat{T}(E, M_1, M_2, M_3) \\ &:= \left(\alpha_1 \mathrm{tr}(M_1 E) + \alpha_2 \mathrm{tr}(M_2 E) + \alpha_3 \mathrm{tr}(M_3 E) \right) M_1 \\ &+ \left(\alpha_2 \mathrm{tr}(M_1 E) + \alpha_1 \mathrm{tr}(M_2 E) + \alpha_3 \mathrm{tr}(M_3 E) \right) M_2 \\ &+ \left(\alpha_3 (\mathrm{tr}(M_1 E) + \alpha_2 \mathrm{tr}(M_2 E)) + \alpha_4 \mathrm{tr}(M_3 E) \right) M_3 \\ &+ \alpha_5 \left((M_1 + M_2) E + E(M_1 + M_2) \right) + \alpha_6 \left(M_3 E + E M_3 \right), \end{split}$$
(21)

where α_j (j = 1, 2, ..., 6) are undetermined coefficients. In the Kelvin notation (see Section 4 below), the elasticity tensor \mathbb{C} that pertains to the stress-strain relation $T = \hat{T}(E, M_1, M_2, M_3)$ in equation (21) is represented by the 6×6 matrix

$$\begin{pmatrix} \alpha_1 + 2\alpha_5 & \alpha_2 & \alpha_3 & 0 & 0 & 0 \\ \alpha_2 & \alpha_1 + 2\alpha_5 & \alpha_3 & 0 & 0 & 0 \\ \alpha_3 & \alpha_3 & \alpha_4 + 2\alpha_6 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_5 + \alpha_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & \alpha_5 + \alpha_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\alpha_5 \end{pmatrix}.$$
 (22)

It is a straightforward matter to verify that the function $\hat{T}(E, M_1, M_2, M_3)$ in equation (21) is isotropic and, by means of equation (20), that

$$\hat{\boldsymbol{T}}(\boldsymbol{E}, \boldsymbol{Q}\boldsymbol{M}_{1}\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}\boldsymbol{M}_{2}\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}\boldsymbol{M}_{3}\boldsymbol{Q}^{\mathrm{T}}) = \hat{\boldsymbol{T}}(\boldsymbol{E}, \boldsymbol{M}_{1}, \boldsymbol{M}_{2}, \boldsymbol{M}_{3}) \quad \text{for each } \boldsymbol{Q} \in \mathcal{G},$$
(23)

which together imply with equation $(21)_1$ that T(E), as given by the representation formula $(21)_2$, indeed satisfies equation (18) with $\mathcal{G} = D_{4h}$. Moreover, as it is clear from the matrix given by equation (22) representing the elasticity tensor \mathbb{C} , every constitutive function T that satisfies equation (18) with $\mathcal{G} = D_{4h}$ has an isotropic extension \hat{T} given by equation (21). Hence $\hat{T}(E, M_1, M_2, M_3)$ as given by equation (21) is a perfectly fine isotropic extension of the tetragonal constitutive function T(E) via the structural tensors M_1, M_2 , and M_3 .

If we further impose on equation (21) the additional conditions that $\alpha_3 = \alpha_2$, $\alpha_4 = \alpha_1$, and $\alpha_6 = \alpha_5$, then the resulting representation formula is an isotropic extension for the stress-strain relation T = T(E) of a cubic material with symmetry group $\mathcal{G} = O_h$. Conversely, the stress-strain relation of any cubic linearly-elastic material can be expressed in the coordinate-free form given by equation (21) with the aforementioned additional conditions on elastic coefficients imposed.

Remark 2.1. In the examples above we have used the method of isotropic extension via structural tensors to derive coordinate-free representation formulas for anisotropic constitutive functions whose symmetry group \mathcal{G} does not keep every structural tensor invariant. Take tetragonal materials with $\mathcal{G} = D_{4h}$ for instance. The symmetry operation $\mathbf{R}(e_3, \pi/2) \in \mathcal{G}$ takes M_1 to M_2, M_2 to M_1 , and preserves only M_3 . But, while $\mathbf{R}(e_3, \pi/2)$ does not keep every structural tensor invariant, it does preserve the isotropic extension function \hat{T} in equations (16) and (21), which is in fact the crucial point at issue. In the formulation of Boehler and Liu, to require that material symmetry be described by the invariance group \mathcal{G}_s of the structural tensors, every element of which should preserve each structural tensor (see definition (3)), is too restrictive and unnecessary. In fact a material point may have several distinguished but equivalent directions, lines, or planes characterized by structural tensors which describe the distinguished but equivalent directions, lines, or planes will not affect material response even if it does not keep each structural tensor invariant. Such an orthogonal transformation should belong to the symmetry group \mathcal{G} of the material. In the original formulation one important role played by the requirement

$$Q\vec{m} = \vec{m}$$
 and $Q\vec{M}Q^{T} = \vec{M}$ for each $Q \in \mathcal{G}_{s}$ (24)

is to guarantee that the isotropic extension satisfies (cf. equations $(7)_2$, (16), and (23))

$$\hat{S}(\vec{v}, \vec{A}, Q\vec{m}, Q\vec{M}Q^{\mathrm{T}}) = \hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M}) \quad \text{for each } Q \in \mathcal{G}$$
(25)

if $\mathcal{G} = \mathcal{G}_s$. As illustrated by the examples presented in this section, requirement (24) is not a necessary condition for the validity of equation (25).

3. Reformulation of the method of isotropic extension

For brevity, in what follows we restrict our discussion to second-order-tensor-valued constitutive functions. The cases of scalar- and vector-valued functions are similar.

Let V be the translation space of the three-dimensional physical space and $V^{\otimes 2} := V \otimes V$ the space of second-order tensors. Let $V^p := V \times V \times \cdots \times V$ (p times) and $(V^{\otimes 2})^q := V^{\otimes 2} \times V^{\otimes 2} \times \cdots \times V^{\otimes 2}$ (q times). Let \mathcal{G} be a subgroup of the orthogonal group O(3). For $\mathbf{v}_i \in V$ (i = 1, ..., p) and $A_j \in V^{\otimes 2}$ (j = 1, ..., q), let $\vec{\mathbf{v}} = (\mathbf{v}_1, ..., \mathbf{v}_p)$ and $\vec{\mathbf{A}} = (\mathbf{A}_1, ..., \mathbf{A}_q)$. Let \mathcal{D} be a domain in $V^p \times (V^{\otimes 2})^q$ that is invariant under the action of O(3), i.e.

$$(\boldsymbol{Q}\boldsymbol{\bar{v}},\boldsymbol{Q}\boldsymbol{\bar{A}}\boldsymbol{Q}^{\mathrm{I}})\in\mathcal{D}$$
 for each $(\boldsymbol{\bar{v}},\boldsymbol{\bar{A}})\in\mathcal{D}$ and $\boldsymbol{Q}\in\mathrm{O}(3)$

Our objective is to find a representation formula for a given class A of anisotropic constitutive functions S: $\mathcal{D} \to V^{\otimes 2}$ that satisfies

$$QS(\vec{v},\vec{A})Q^{\mathrm{T}} = S(Q\vec{v},Q\vec{A}Q^{\mathrm{T}}) \quad \text{for each } Q \in \mathcal{G},$$
⁽²⁶⁾

where

$$\boldsymbol{Q}\boldsymbol{\vec{v}} := (\boldsymbol{Q}\boldsymbol{v}_1, ..., \boldsymbol{Q}\boldsymbol{v}_p), \qquad \boldsymbol{Q}\boldsymbol{\vec{A}}\boldsymbol{Q}^{\mathrm{T}} := (\boldsymbol{Q}\boldsymbol{A}_1\boldsymbol{Q}^{\mathrm{T}}, ..., \boldsymbol{Q}\boldsymbol{A}_q\boldsymbol{Q}^{\mathrm{T}}).$$
(27)

To this end, we reformulate the method of isotropic extension via structural tensors as follows: Seek specific structural vectors $\mathbf{m}_1, \ldots, \mathbf{m}_r$ and/or second-order tensors M_1, \ldots, M_s , and a class Ext of functions $\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$ with domain

$$\mathcal{D} \times O(\mathbf{m}_1) \times \cdots \times O(\mathbf{m}_r) \times O(\mathbf{M}_1) \times \cdots \times O(\mathbf{M}_s)$$

where \vec{m} and \vec{M} are defined in equation (1), and

$$O(\boldsymbol{m}_k) = \{\boldsymbol{Q}\boldsymbol{m}_k : \boldsymbol{Q} \in O(3)\}, \quad (k = 1, \dots, r)$$
$$O(\boldsymbol{M}_l) = \{\boldsymbol{Q}\boldsymbol{M}_l \boldsymbol{Q}^{\mathrm{T}} : \boldsymbol{Q} \in O(3)\}, \quad (l = 1, \dots, s)$$

.

.

are the orbits of m_k and M_l under O(3), respectively, such that

1. For each $S \in A$, there is an $\hat{S} \in Ext$ which is an extension of S in the sense that

$$\widehat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M}) = S(\vec{v}, \vec{A})$$
(28)

for each (\vec{v}, \vec{A}) in the domain \mathcal{D} of S.

2. $\hat{\boldsymbol{S}}$ is isotropic, i.e.

$$\hat{S}(\boldsymbol{Q}\boldsymbol{\vec{v}},\boldsymbol{Q}\boldsymbol{\vec{A}}\boldsymbol{Q}^{\mathrm{T}},\boldsymbol{Q}\boldsymbol{\vec{m}},\boldsymbol{Q}\boldsymbol{\vec{M}}\boldsymbol{Q}^{\mathrm{T}}) = \boldsymbol{Q}\hat{S}(\boldsymbol{\vec{v}},\boldsymbol{\vec{A}},\boldsymbol{\vec{m}},\boldsymbol{\vec{M}})\boldsymbol{Q}^{\mathrm{T}}$$
(29)

for each $Q \in O(3)$.

3. For each $(\vec{v}, \vec{A}) \in \mathcal{D}$, the function $\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$ satisfies

$$\hat{S}(\vec{v}, \vec{A}, Q\vec{m}, Q\vec{M}Q^{\mathrm{T}}) = \hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$$
(30)

for each $Q \in G$.

Note that in the reformulation above, the symmetry group \mathcal{G} of the material is not determined by the overly restrictive requirement given by equation (3) that its elements keep each structural tensor invariant, which leads to the limitations of the formulation of Boehler and Liu. Here the group \mathcal{G} , the anisotropic S, the isotropic extension \hat{S} , and the structural tensors are interrelated through equations (26), (28), and (30).

For a constitutive function $S(\vec{v}, \vec{A})$, if we can find structural vectors \boldsymbol{m}_k (k = 1, ..., r) and/or second-order tensors \boldsymbol{M}_l (l = 1, ..., s) and an isotropic extension $\hat{\boldsymbol{S}}$ of \boldsymbol{S} such that the conditions given by equations (28) to (30) hold, then for each $\boldsymbol{Q} \in \mathcal{G}$ we have

$$S(Q\vec{v}, Q\vec{A}Q^{T}) = \hat{S}(Q\vec{v}, Q\vec{A}Q^{T}, \vec{m}, \vec{M})$$

= $\hat{S}(Q\vec{v}, Q\vec{A}Q^{T}, Q\vec{m}, Q\vec{M}Q^{T})$
= $Q\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})Q^{T}$
= $QS(\vec{v}, \vec{A})Q^{T}$. (31)

Thus S has anisotropy characterized by the group G.

On the other hand, given a constitutive function S with anisotropy described by group \mathcal{G} , whether there exists an isotropic extension \hat{S} with structural vectors and/or second-order tensors that satisfy the conditions given by equations (28) to (30) above remains to be investigated.

4. Anisotropic linear elasticity

The simple example of anisotropic linear elasticity offers a glimpse of what could happen under the reformulation. Let e_i (i = 1, 2, 3) be a right-handed orthonormal triad of vectors in V. Let

$$M_{1} = e_{1} \otimes e_{1}, \quad M_{2} = e_{2} \otimes e_{2}, \quad M_{3} = e_{3} \otimes e_{3}, \quad M_{4} = \frac{1}{\sqrt{2}}(e_{2} \otimes e_{3} + e_{3} \otimes e_{2}),$$
$$M_{5} = \frac{1}{\sqrt{2}}(e_{3} \otimes e_{1} + e_{1} \otimes e_{3}), \quad M_{6} = \frac{1}{\sqrt{2}}(e_{1} \otimes e_{2} + e_{2} \otimes e_{1}).$$
(32)

Let Sym be the linear space of second-order symmetric tensors. For two tensors $A, B \in Sym$, let $A \cdot B := tr(AB)$ denote the inner product of A and B in Sym. Under this inner product, the tensors M_{α} ($\alpha = 1, 2, ..., 6$) constitute an orthonormal basis in Sym. Let \mathbb{C} : Sym \rightarrow Sym be the fourth-order elasticity tensor; it is a symmetric linear transformation on Sym. In the Kelvin notation [10], the Cauchy stress T and the infinitesimal strain E are treated as 6-dimensional vectors in Sym, and the elasticity tensor \mathbb{C} as a symmetric second-order tensor in Sym \otimes Sym

$$T = \sum_{\alpha=1}^{6} (T \cdot M_{\alpha}) M_{\alpha}, \qquad E = \sum_{\alpha=1}^{6} (E \cdot M_{\alpha}) M_{\alpha}, \qquad (33)$$

$$\mathbb{C} = \sum_{\alpha,\beta=1}^{6} c_{\alpha\beta} M_{\alpha} \otimes M_{\beta}, \quad \text{where } c_{\alpha\beta} = c_{\beta\alpha} = M_{\alpha} \cdot \mathbb{C}[M_{\beta}].$$
(34)

Note that $c_{\alpha\beta}$ are the entries of the 6 × 6 matrix that represents the elasticity tensor \mathbb{C} under the basis M_{α} ($\alpha = 1, 2, ..., 6$). Since they are inner products, their values are independent of the choice of Cartesian coordinate system in V.

The stress-strain relation $T = T(E) = \mathbb{C}[E]$ of a generally-anisotropic linearly-elastic material can be written in the following coordinate-free form

$$T(E) = T(E, M_1, M_2, \dots, M_6)$$

$$:= \left(\sum_{\alpha, \beta=1}^{6} c_{\alpha\beta} M_{\alpha} \otimes M_{\beta}\right) \left[\sum_{\gamma=1}^{6} (E \cdot M_{\gamma}) M_{\gamma}\right]$$

$$= \sum_{\alpha, \beta, \gamma=1}^{6} c_{\alpha\beta} \delta_{\beta\gamma} (E \cdot M_{\gamma}) M_{\alpha} = \sum_{\alpha, \beta=1}^{6} c_{\alpha\beta} \operatorname{tr}(M_{\beta} E) M_{\alpha}, \qquad (35)$$

which is just an expression of the constitutive equation $T = \mathbb{C}[E]$ under the basis $\{M_{\alpha} : \alpha = 1, 2, ..., 6\}$. Clearly $\hat{T}(E, M_1, M_2, ..., M_6)$ is an isotropic extension of the anisotropic T(E) via six structural tensors M_1 , $M_2, ..., M_6$. From the theory of anisotropic linear elasticity we know that, by putting suitable restrictions on the elastic constants $c_{\alpha\beta}$, constitutive equation $T = \mathbb{C}[E]$ with material symmetry characterized by any of the 32 crystallographic point groups and five transversely-isotropic limit groups can be put in the form of equation (35). For instance, to get a representation formula for the class of tetragonal linearly-elastic materials discussed in Section 2, we just need to put $c_{11} = c_{22}$, $c_{13} = c_{23}$, $c_{44} = c_{55}$, keep in addition c_{12} , c_{33} , c_{66} , and set all other elastic constants zero. The resulting representation formula is

$$T(E) = \tilde{T}(E, M_1, M_2, \dots, M_6)$$

$$:= (c_{11} \operatorname{tr}(M_1 E) + c_{12} \operatorname{tr}(M_2 E) + c_{13} \operatorname{tr}(M_3 E)) M_1$$

$$+ (c_{12} \operatorname{tr}(M_1 E) + c_{11} \operatorname{tr}(M_2 E) + c_{13} \operatorname{tr}(M_3 E)) M_2$$

$$+ (c_{13} (\operatorname{tr}(M_1 E) + c_{13} \operatorname{tr}(M_2 E)) + c_{33} \operatorname{tr}(M_3 E)) M_3$$

$$+ c_{44} (\operatorname{tr}(M_4 E)) M_4 + \operatorname{tr}(M_5 E)) M_5) + c_{66} \operatorname{tr}(M_6 E)) M_6.$$
(36)

Thus, as shown by the example of anisotropic linear elasticity, under our present reformulation it is possible that the method of isotropic extension could cover anisotropic constitutive functions with anisotropy defined by any of the 32 crystallographic point groups and five transversely-isotropic limit groups with isotropic extension functions involving only structural tensors of order not higher than two.

Remark 4.1. The original formulation of isotropic extension restricts attention to invariance groups of structural tensors, which define the particular directions, lines, or planes that characterize the anisotropy in question. Our reformulation relaxes this restriction, which opens the door to our using of M_{α} ($\alpha = 1, ..., 6$) as structural tensors that cover at once all the aforementioned 37 groups of material symmetry. On one hand, in equation (35) with the appropriate restrictions on elastic constants we have obtained a coordinate-free representation formula which is an isotropic extension of the corresponding constitutive function for each of the aforementioned types

of anisotropy. On the other hand, the geometric properties associated with these structural tensors no longer have a clear cut connection to the geometric properties that are invariant under the symmetry group associated with the anisotropy. \Box

Remark 4.2. In the original formulation of Boehler and Liu, the structural tensors for isotropic extension must be chosen so that the invariance group \mathcal{G}_s of the structural tensors is the symmetry group of the anisotropic constitutive function in question. An over-prescription of structural tensors can easily reduce the invariance group to the cases $\mathcal{G}_s = \{I\}$ or $\{I, -I\}$. However, over-prescription of structural tensors is allowed in the proposed reformulation. For instance, for anisotropic linear elasticity, the invariance group of the structural tensors M_{α} ($\alpha = 1, \ldots, 6$) is $\mathcal{G}_s = \{I, -I\}$, a case of triclinic symmetry. By imposing suitable restrictions on elastic constants in (35), we have used M_{α} ($\alpha = 1, \ldots, 6$) as structural tensors for isotropic extension of linearly-elastic constitutive functions for crystals and materials with symmetry characterized by any of the 32 crystallographic point groups and five transversely-isotropic limit groups.

In general, representation formulas should be as simple and elegant as possible. Here representation formula (36) involves six structural tensors, whereas its alternate counterpart given by equation (21) carries only three, namely $M_1 = e_1 \otimes e_1$, $M_2 = e_2 \otimes e_2$ and $M_3 = e_3 \otimes e_3$, where e_1 and e_2 define two 2-fold axes of rotational symmetry, and e_3 a 4-fold axis of symmetry for the tetragonal material in question. While the discussion above indicates that our proposed reformulation of the method of isotropic extension provides a coordinate-free representation for each type of linear-elastic anisotropy, work remains to be done to complete the list of irreducible representations.

5. Concluding remarks

With the objective to derive coordinate-free representation formulas for anisotropic constitutive functions such as $S(\vec{v}, \vec{A})$ with anisotropy characterized by a subgroup \mathcal{G} of O(3) in the sense of equation (4), both Boehler [4] and Liu [5] begin by restricting attention to the cases where \mathcal{G} is an invariance group \mathcal{G}_s of structural tensors, i.e. it renders each member of a finite list of structural vectors \vec{m} and/or second-order structural tensors \vec{M} invariant. Liu proves that there exists an isotropic extension $\hat{S}(\vec{v}, \vec{A}, \vec{m}, \vec{M})$ of any anisotropic $S(\vec{v}, \vec{A})$ whose symmetry group $\mathcal{G} = \mathcal{G}_s$, an invariance group of structural tensors. Representation theorems for isotropic functions can then be used to obtain coordinate-free representation formulas for the isotropic \hat{S} and thus also the anisotropic S. This is the method of isotropic extension via structural tensors as originally formulated by Boehler and by Liu. Unfortunately, as pointed out by Xiao et al. [9], only cylindrical groups and those in the triclinic, monoclinic, or rhombic crystal classes can be taken as invariance groups of structural tensors of order not higher than two.

In this paper, we present examples in finite and linear elasticity where we derive formulas for an isotropic extension of constitutive functions with symmetry group that is tetragonal (D_{4h}) or octahedral (O_h) . Either of these is not an invariance group of structural tensors of order not higher than two. These derivations suggest a reformulation of the method of isotropic extension, in which we replace the assumption on symmetry group \mathcal{G} , namely that it is some invariance group \mathcal{G}_s of structural tensors, by the condition given by equation (30) on the invariance of \hat{S} under the action of \mathcal{G} on the structural tensors. We show by example of anisotropic linear elasticity, that under the reformulation isotropic extension of the stress-strain relation, T = T(E) is possible for material symmetry characterized by any of the 32 crystallographic point groups and five transversely-isotropic limit groups. However, in general, the existence of isotropic extension for anisotropic constitutive functions, which is guaranteed by Liu's theorem when the symmetry group \mathcal{G} is an invariance group \mathcal{G}_s of structural tensors, remains an open problem when $\mathcal{G} \neq \mathcal{G}_s$.

The method of isotropic extension via structural tensors gives only a general procedure in outline. In applications, for each class of anisotropic constitutive functions with a specific material symmetry group \mathcal{G} , suitable structural tensors have to be selected to begin with. Application of representation theorems for isotropic functions to get isotropic extensions will usually lead to formulas that are not irreducible. Using this method to obtain irreducible representation formulas for anisotropic constitutive functions will require laborious work in each specific case.

Notes

- 1. Liu [5] in fact formulates his theory in a more general setting. In the definition given by equation (3) for \mathcal{G}_s he puts $Q \in G$, where *G* is a given subgroup of O(3), although he restricts attention to G = O(3) or G = SO(3) (i.e. the rotation group) in specific developments of the theory. In this paper we are interested only in isotropic extensions and take G = O(3).
- 2. For the case where the independent variables of S and the structural tensors are objective or frame-indifferent [7], Boehler [4] appeals to the principle of material frame-indifference to justify this requirement on the isotropy of \hat{S} . This justification is based on the assumption that $\vec{v}, \vec{A}, \vec{m}$, and \vec{M} include all "agencies" that affect the material response, which presumably are represented by tensors associated with the current configuration of the material.

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