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LARGE STRAIN INELASTIC STATE VARIABLE THEORY

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Abstract—A precise format for the construction of three-dimensional, large strain inelastic state variable models through the continuum modeling of micromechanism is proposed. This general theory is based on a concept of state wherein each material element in its present configuration is regarded as a "black box" which converts possible future stimuli (deformations) into future response (stress and internal energy). Fundamental considerations suggest that state is determined by the instantaneous spatial distribution of the material bonds. The parameterization of the accessible states with N-tuples of tensor state variables is considered and the explicit assumptions which make it possible to reduce causal functional forms to response and incremental evolution equations are enumerated. The specific restrictions associated with material frame invariance and material symmetry are specified at each step of this development. The presentation concludes by considering some important specialized theories which contain virtually all successful models in the field of inelasticity.

1. INTRODUCTION

The recognized inadequacy of the classical theories in many sensitive applications, such as the design of turbine and nuclear reactor components, has spurred considerable interest in the development of new, large deformation constitutive models for the inelastic response of metals. Important recent contributions in this area have come from the materials science community through the proposal of a number of state variable models (e.g. [1–3]). A principal characteristic of these models is that the accumulated effect of deformation history on future material response is fully characterized by the current values assigned to a finite collection of state variables which are, in some manner, descriptive of the instantaneous material microstructure. This approach to materials modeling is philosophically distinct from (but not necessarily incompatible with) the traditional mechanics approach which tends to emphasize purely kinematic concepts such as deformation history and "remembered" element configurations. A similar dichotomy of philosophical perspective exists between the chemical rheologists and the "simple fluid" mechanists in the modeling of non-Newtonian fluids.

The purpose of this paper is to establish a mechanistically sound, alternative theoretical structure for the modeling of inelastic solids which accommodates the microstructural approach in a more natural fashion. The theoretical foundation for this theory is based on a concept of "state" which is consonant with an emergent trend away from infinite history/fading memory formalisms. Within the present context, state is best described as the collection of all things, including the present configuration, past history and inherent physical properties, which serve to distinguish one material element from another. Fundamental considerations suggest that knowledge of state should follow from the specification of chemical composition and a detailing of the instantaneous spatial distribution of material bonds. The present state of a material element is considered to determine the class of possible future stimuli (deformations), as well as the subsequent "response" (stress and free energy) to each through a response functional. In addition, the evolution of element state as it accumulates additional experience (history) during an ongoing deformation process is described in terms of a state evolution functional. These constructs, as well as precise statements of the principles of determinism and material frame invariance, are mathematically formalized in Section 2.

Section 3 deals with the "modeling" of state for solid-like material elements through

the introduction of internal variables as state descriptors. The structural regularity of crystalline solids is exploited by selecting a cubic reference cell to serve as a model (or map) of the characteristic bond structure of the material under consideration. Having established such a cell as a standard for comparison, the linear transformation (the so-called "cell placement tensor") which "places" this characteristic cell in the present configuration is adopted as a primitive descriptor of the instantaneous state. This distinctive use of the reference concept serves to emphasize the present focus on microstructure as opposed to kinematics. Simply put, physical significance is ascribed to the spatial distribution of bonds, not the spatial distribution of material relative to a chosen reference. This is the fundamental feature which distinguishes this constitutive format.

Although reference cell placement is intended to provide a statistically "accurate" picture of the instantaneous bond structure, the presence of structural dislocations can give rise to physically significant perturbations which may alter the elastic properties as well as the inelastic flow characteristics. Thus, provision is made for the introduction of a finite number of dislocation state variables. No attempt is made to define these variables beyond the suggestion that they be statistically descriptive (in a geometric sense) of the instantaneous spatial distributions of the different types of structural dislocations.

Having thus modeled the state space as a finite dimensional manifold, the general functional forms of Section 2 are recast in terms of the state descriptors. This process is not as direct as it might first appear due to the possibility of structural symmetry which would effectively partition the cell placement tensors into nontrivial equivalence classes of indistinguishable elements. These considerations lead to state variable response and evolution functionals which are constrained not only by frame invariance and "consistency" requirements, but also by structural symmetry requirements phrased in terms of the orthogonal symmetry group associated with the chosen reference cell. Additional assumptions relating to the "smoothness" properties of these functionals are then shown to justify their replacement with more familiar response functions and differential rate equations governing the evolution of the state variables.

A distinctive feature of this general theory is that it is formulated in a spatial or Eulerian (as opposed to a referential or Lagrangian) context in which all response variables and state descriptors are defined and interpreted in the current element configuration. In fact, since a fixed material reference (as opposed to a bond reference) plays no role in this formulation, total strain measures are eliminated altogether. These features give rise to relatively compact incremental constitutive forms of the type more familiar to fluid rheologists. In this regard it is curious that while Lagrangian formulations are dominant in the field of large deformation inelasticity, they are universally rejected in the modeling of fluids—this despite the fact that most inelastic deformation mechanisms are "fluidic" in nature.

The final section serves to demonstrate the utility of this nonstandard large deformation constitutive format. In part A, thermodynamic restrictions are imposed on the class of elastic solids (both isotropic and anisotropic) in order to establish the appropriate constitutive relations for hyperelasticity, large strain viscoelasticity, and the approximate forms for "small strain on large". In part B, the introduction of a "dislocation strain" tensor and the formulation of a corresponding general theory illustrate a phenomenological approach to the modeling of dislocation distribution. This specialized theory, despite its simplicity, is of interest inasmuch as it contains virtually all widely used inelastic models as special cases. In particular, this theory is shown to encompass isotropic hyperelasticity as well as large strain generalizations of the classical isotropic and kinematic hardening elastic-plastic models, and a recently proposed, rate sensitive, state variable model based on the notion of "anelastic" strain.

2. THEORETICAL FOUNDATION

Before fixing a theoretical structure for the modeling of inelastic solids it is necessary to establish an axiomatic foundation for constitutive theory which is not constrained by a "fading memory" requirement. A general constitutive format based on an emergent concept

of "state", variants of which have been proposed by Noll[4] and Bertram[5], is adopted for the present development.

The symbol Σ shall be used to denote the instantaneous "state" of a material element. The *state* of a material element is regarded as the embodiment of the intrinsic material properties as well as all past experience up to and including the instantaneous spatial placement. In principle, knowledge of state would follow from a "detailing" of the instantaneous spatial distribution of molecular bonds in the immediate neighborhood of the element location.

The state of a material element at time t, Σ_t, is assumed to establish the set of possible future deformations, or *stimuli*, as well as the subsequent *response* to each through a *response functional* $\mathscr{R}$. Using the symbol $\boldsymbol{R}$ to represent the mechanical response pair (σ, ψ) consisting of Cauchy (true) stress σ and free energy density ψ, and the notation

$$\mathbf{F}_\tau^t = \{[s, \mathbf{F}(s)] : t < s \leqslant \tau\}; \qquad \tau > t \tag{2.1}$$

to represent an "admissible" future stimulus expressed in terms of the local deformation gradient $\mathbf{F}$ measured relative to the time t element configuration, this supposition takes the mathematical form

$$\boldsymbol{R}(\tau) = \mathscr{R}[\Sigma_t ; \mathbf{F}_\tau^t]. \tag{2.2}$$

With this, the usual axiomatic statements pertaining to determinism and causality can be compressed into the assertion that every material element, at each moment of its existence, has a state. Moreover, in view of the aforementioned constituents of state, the existence of a *state evolution functional* $\mathscr{E}$, which serves to "update" an element's state through an expression of the form

$$\Sigma_\tau = \mathscr{E}[\Sigma_t ; \mathbf{F}_\tau^t], \tag{2.3}$$

can be inferred.

These functionals must, of course, be subject to the restrictions associated with the axiom of invariance of frame. This axiom asserts that, insofar as material response is concerned, space is not only homogeneous but also isotropic. Spatial homogeneity is, in fact, implicit in the functional forms (2.2) and (2.3) due to the fact that spatial position has been ignored in the description of stimulus. In order to formalize the notion of spatial isotropy let $\mathrm{T}_\mathbf{Q}\boldsymbol{R}$ and $T_\mathbf{Q}\Sigma$ represent the transformed element response $\boldsymbol{R}$ and state Σ resulting from the instantaneous element reorientation associated with the proper orthogonal rotation tensor $\mathbf{Q}$, i.e.

$$\begin{aligned} \boldsymbol{R} = (\sigma, \psi) \to \mathrm{T}_\mathbf{Q}\boldsymbol{R} = (\mathbf{Q}\sigma\mathbf{Q}^T, \psi) \\ \Sigma \to T_\mathbf{Q}\Sigma. \end{aligned} \tag{2.4}$$

With the introduction of the Green deformation tensor

$$\mathbf{C} \equiv \mathbf{F}^T\mathbf{F}, \tag{2.5}$$

and the additional notation

$$\mathbf{C}_\tau^t \equiv \{[s, \mathbf{C}(s)] : t < s < \tau\}, \tag{2.6}$$

the axiom of *frame invariance* can be stated as follows :

> Given the state Σ_t of a material element at time t, the future state/response depend on subsequent element orientations only through its terminal value, and then only

insofar as it serves to "orient" the resultant state/response, i.e.

$$\begin{aligned} \boldsymbol{R}(\tau) &= \mathscr{R}[\Sigma_t, \mathbf{F}(\tau); \mathbf{C}_\tau^t], \\ \Sigma_\tau &= \mathscr{E}[\Sigma_t, \mathbf{F}(\tau); \mathbf{C}_\tau^t]; \qquad \tau > t \end{aligned} \tag{2.7}$$

subject to

$$\begin{aligned} \mathrm{T}_{\mathbf{Q}}\boldsymbol{R}(\tau) &= \mathscr{R}[\Sigma_t, \mathbf{QF}(\tau); \mathbf{C}_\tau^t], \\ T_{\mathbf{Q}}\Sigma_\tau &= \mathscr{E}[\Sigma_t, \mathbf{QF}(\tau); \mathbf{C}_\tau^t]; \qquad \tau > t \end{aligned} \tag{2.8}$$

for all proper orthogonal $\mathbf{Q}$.

The general constitutive forms in (2.7), subject to frame invariance through (2.8), establish a suitable foundation for the modeling of materials, such as inelastic solids, which are not characterized by the property of fading memory.

Before proceeding to specialize these forms it should be evident that the response and evolution functionals must satisfy certain *consistency* conditions. In terms of any admissible stimulus

$$\mathbf{F} = \mathbf{F}(s): t < s \leq \tau; \qquad \tau > t$$

measured relative to the time t element configuration, it is clearly necessary to require that both functionals satisfy

$$\mathscr{H}[\Sigma_t, \mathbf{F}(\tau); \mathbf{C}_\tau^t] = \mathscr{H}\{\Sigma_\eta, \mathbf{F}(\tau)\mathbf{F}^{-1}(\eta); [\mathbf{F}^{-1}(\eta)]^T \mathbf{C}_\tau^\eta \mathbf{F}^{-1}(\eta)\}, \tag{2.9}$$

with

$$\Sigma_\eta = \mathscr{E}[\Sigma_t, \mathbf{F}(\eta); \mathbf{C}_\eta^t],$$

for any η such that $t < \eta < \tau$. In particular, by considering a stimulus that initiates with an instantaneous rigid rotation it necessarily follows that $\eta = t^+, \Sigma_\eta = T_{\mathbf{Q}}\Sigma_t, \mathbf{F}(\eta) = \mathbf{Q}$, and

$$\mathscr{H}[\Sigma_t, \mathbf{F}(\tau); \mathbf{C}_\tau^t] = \mathscr{H}[T_{\mathbf{Q}}\Sigma_t, \mathbf{F}(\tau)\mathbf{Q}^T; \mathbf{QC}_\tau^t\mathbf{Q}^T] \tag{2.10}$$

for all proper orthogonal $\mathbf{Q}$. Combination of this consistency condition with frame invariance, through (2.8), results in the additional "tensor transformation" requirements

$$\begin{aligned} \mathrm{T}_{\mathbf{Q}}\boldsymbol{R}(\tau) &= \mathscr{R}[T_{\mathbf{Q}}\Sigma_t, \mathbf{QF}(\tau)\mathbf{Q}^T; \mathbf{QC}_\tau^t\mathbf{Q}^T], \\ T_{\mathbf{Q}}\Sigma_\tau &= \mathscr{E}[T_{\mathbf{Q}}\Sigma_t, \mathbf{QF}(\tau)\mathbf{Q}^T; \mathbf{QC}_\tau^t\mathbf{Q}^T], \end{aligned} \tag{2.11}$$

for all proper orthogonal $\mathbf{Q}$.

One final consideration relates to the "continuation" characteristics of the set of allowable future stimuli and the smoothness properties of the above response and evolution functionals. Suppose, for example, that the set of allowable stimuli contains the subset of all C_K (K-times continuously differentiable) deformation processes. If this is the case then any C_K deformation process

$$\mathbf{F} = \mathbf{F}_1(t-s); \qquad s \geqslant 0$$

can be continued beyond time t with the "polynomic" extension

$$\mathbf{F} = \mathbf{F}_2(t+s) = \mathbf{R}(t+s)\left[\sum_{n=0}^{K} \frac{1}{n!}\mathbf{A}_n(t^-)s^n\right]^{1/2}\mathbf{F}_1(t); \qquad s > 0, \tag{2.12}$$

expressed in terms of the symmetric Rivlin–Ericksen tensors

$$\begin{aligned} \mathbf{A}_0 &= \mathbf{I}, \\ \mathbf{A}_1 &= 2\mathbf{D}, \\ \mathbf{A}_{n+1} &= \dot{\mathbf{A}}_n + \mathbf{A}_n\mathbf{L} + \mathbf{L}^T\mathbf{A}_n; \qquad n = 0, 1, \ldots, \end{aligned} \tag{2.13}$$

and any smooth proper orthogonal orientation extension $\mathbf{R}(t+s)\colon s > 0$, subject to

$$\begin{aligned} \mathbf{I} &= \lim_{s\to 0} \mathbf{R}(t+s), \\ \mathbf{W}(t^-) &= \lim_{s\to 0} \{\dot{\mathbf{R}}(t+s)\mathbf{R}^T(t+s)\}. \end{aligned} \tag{2.14}$$

In these expressions the symbols $\mathbf{L}$, $\mathbf{D}$ and $\mathbf{W}$ have been introduced to represent the velocity gradient tensor

$$\mathbf{L} = \nabla \mathbf{v} = \dot{\mathbf{F}}\mathbf{F}^{-1}, \tag{2.15}$$

and its symmetric and antisymmetric rate of deformation and vorticity components

$$\begin{aligned} \mathbf{D} &= \tfrac{1}{2}(\mathbf{L} + \mathbf{L}^T), \\ \mathbf{W} &= \tfrac{1}{2}(\mathbf{L} - \mathbf{L}^T). \end{aligned} \tag{2.16}$$

Given this continuation property, consider now a functional of the form

$$\tilde{\mathbf{m}}(\tau) = \mathscr{M}[\Sigma_t, \mathbf{F}(\tau);\, \mathbf{C}_\tau^t]; \qquad \tau > t \tag{2.17}$$

governing the evolution of some tensor variable $\tilde{\mathbf{m}}$, subject to the consistency condition (2.9) and invariance through

$$\mathrm{T}_{\mathbf{Q}}\tilde{\mathbf{m}}(\tau) = \begin{cases} \mathscr{M}[\Sigma_t, \mathbf{QF}(\tau);\, \mathbf{C}_\tau^t] \\ \mathscr{M}[T_{\mathbf{Q}}\Sigma_t, \mathbf{QF}(\tau)\mathbf{Q}^T;\, \mathbf{QC}_\tau^t\mathbf{Q}^T]; \qquad \tau > t \end{cases} \tag{2.18}$$

for arbitrary proper orthogonal $\mathbf{Q}$. If $\tilde{\mathbf{m}}$ is known to evolve continuously under C_K stimuli then any ongoing C_K stimulus leading up to time t can be extended beyond t, as per (2.12), resulting in the continuous $\tilde{\mathbf{m}}$-extension

$$\tilde{\mathbf{m}}(t+s) = \mathscr{M}[\Sigma_t, \mathbf{R}(t+s)\mathbf{C}^{1/2}(t+s);\, \mathbf{C}_{t+s}^t] \tag{2.19}$$

in terms of

$$\mathbf{C}(t+s) = \sum_{n=0}^{K} \frac{1}{n!}\mathbf{A}_n(t^-)s^n; \qquad s > 0,$$

and a smooth orientation extension consistent with (2.14). In view of $(2.18)_1$, $(2.14)_1$, and the continuity property

$$\lim_{s\to 0} \tilde{\mathbf{m}}(t+s) = \tilde{\mathbf{m}}(t),$$

it immediately follows that

$$\begin{aligned} \mathrm{T}_{\mathbf{R}^T(t+s)}\tilde{\mathbf{m}}(t+s) &= \hat{\mathscr{M}}[\Sigma_t, \mathbf{A}_1(t), \ldots, \mathbf{A}_K(t), s], \\ &\equiv \mathscr{M}[\Sigma_t, \mathbf{C}^{1/2}(t+s);\, \mathbf{C}_{t+s}^t], \end{aligned} \tag{2.20}$$

and consequently

$$\begin{aligned}\tilde{\mathbf{m}}(t) &= M[\boldsymbol{\Sigma}_t, \mathbf{A}_1(t), \ldots, \mathbf{A}_K(t)] \\ &\equiv \lim_{s\to 0}\{\hat{\mathscr{M}}[\boldsymbol{\Sigma}_t, \mathbf{A}_1(t), \ldots, \mathbf{A}_K(t), s]\}.\end{aligned} \tag{2.21}$$

Thus, during an ongoing C_K stimulus, the instantaneous value of $\tilde{\mathbf{m}}$ is necessarily determined as a function of the instantaneous state and the first K Rivlin–Ericksen tensors.

By making use of $(2.18)_2$ and the definitions (2.20, 21), it similarly follows that

$$\begin{aligned}\mathrm{T}_{\mathbf{Q}}[\mathrm{T}_{\mathbf{R}^T(t+s)}\tilde{\mathbf{m}}(t+s)] &= \mathscr{M}[T_{\mathbf{Q}}\boldsymbol{\Sigma}_t, \mathbf{Q}\mathbf{C}^{1/2}(t+s)\mathbf{Q}^T; \mathbf{Q}\mathbf{C}^t_{t+s}\mathbf{Q}^T] \\ &= \hat{\mathscr{M}}[T_{\mathbf{Q}}\boldsymbol{\Sigma}_t, \mathbf{Q}\mathbf{A}_1(t)\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K(t)\mathbf{Q}^T, s],\end{aligned} \tag{2.22}$$

and hence

$$\mathrm{T}_{\mathbf{Q}}\tilde{\mathbf{m}}(t) = M[T_{\mathbf{Q}}\boldsymbol{\Sigma}_t, \mathbf{Q}\mathbf{A}_1(t)\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K(t)\mathbf{Q}^T] \tag{2.23}$$

for arbitrary proper orthogonal $\mathbf{Q}$.

From (2.22) it is also evident that if $\tilde{\mathbf{m}}$ evolves smoothly in response to C_K stimuli then

$$\mathrm{T}_{\mathbf{Q}}\mathring{\tilde{\mathbf{m}}}(t) = N[T_{\mathbf{Q}}\boldsymbol{\Sigma}_t, \mathbf{Q}\mathbf{A}_1(t)\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K(t)\mathbf{Q}^T] \tag{2.24}$$

for proper orthogonal $\mathbf{Q}$, where

$$\mathring{\tilde{\mathbf{m}}}(t) \equiv \lim_{s\to 0}\left\{\frac{\mathrm{d}}{\mathrm{d}s}[\mathrm{T}_{\mathbf{R}^T(t+s)}\tilde{\mathbf{m}}(t+s)]\right\}$$

and (2.25)

$$N[\boldsymbol{\Sigma}_t, \mathbf{A}_1(t), \ldots, \mathbf{A}_K(t)] \equiv \lim_{s\to 0}\left\{\frac{\mathrm{d}}{\mathrm{d}s}\hat{\mathscr{M}}[\boldsymbol{\Sigma}_t, \mathbf{A}_1(t), \ldots, \mathbf{A}_K(t), s]\right\}.$$

In view of the limit conditions (2.14) it is a simple exercise to establish the correspondence between the $(\mathring{\ })$ derivative defined above and the corotational or Jaumann time derivative. Consider, for example, the Cauchy stress tensor $\boldsymbol{\sigma}$ and note that

$$\begin{aligned}\mathring{\boldsymbol{\sigma}}(t) &= \lim_{s\to 0}\left\{\frac{\mathrm{d}}{\mathrm{d}s}[\mathrm{T}_{\mathbf{R}^T(t+s)}\boldsymbol{\sigma}(t+s)]\right\} \\ &= \lim_{s\to 0}\left\{\frac{\mathrm{d}}{\mathrm{d}s}[\mathbf{R}^T(t+s)\boldsymbol{\sigma}(t+s)\mathbf{R}(t+s)]\right\} \\ &= \lim_{s\to 0}\{\mathbf{R}^T[\dot{\boldsymbol{\sigma}}+\boldsymbol{\sigma}(\dot{\mathbf{R}}\mathbf{R}^T)-(\dot{\mathbf{R}}\mathbf{R}^T)\boldsymbol{\sigma}]\mathbf{R}\} \\ &= \dot{\boldsymbol{\sigma}}+\boldsymbol{\sigma}\mathbf{W}-\mathbf{W}\boldsymbol{\sigma}.\end{aligned}$$

As will soon become evident, these smoothness properties are crucial to the establishment of the incremental forms generally associated with the "state variable" format.

3. STATE VARIABLE FORMAT

A. *State variables*

This section expands on the particular circumstance wherein the accessible states for a given material are in one-to-one correspondence with the points in a Cartesian product space of N (a finite number) tensor state variables. In principle, one would believe this to

always be possible in view of the fact that knowledge of the precise spatial positions for each of the finite number of atoms in the "effective" neighborhood of a given point would certainly determine the local state. In practice, state variables are most often introduced during the modeling process in which "hypothetical" materials having relatively simple state variable descriptions are defined. Such models are introduced in the hope that their behavior will "closely" approximate, and thus provide a mathematical analog for, the behavior of some real material under a definable range of circumstances. The goal here is to establish a general state variable format which is concordant with the physics of the class of highly structured materials which are generally referred to as solids. Accordingly, attention shall henceforth be restricted to materials for which the spatial description of atomic distribution is simplified by its regularity. Such materials are distinguished by the property that their constituent atoms are always distributed in a particular (perhaps anisotropic) array, perturbed only by a locally linear (but perhaps finite) elastic distortion of the characteristic lattice or cell structure and a statistically small (but perhaps important) number of cell dislocations.

In view of the foregoing remarks, the state variables for a particular material model should be selected so as to provide the "best picture" of the instantaneous local bond structure. With this in mind, the structural regularity of solids may best be exploited by selecting the *cell placement tensor* $\mathbf{F}_e$ as a primary state variable. Having chosen and set aside a particular "virgin" element of this material, $\mathbf{F}_e$ is defined as the proper nonsingular deformation gradient tensor which "places" this characteristic lattice or cell in the deformed material element, thus providing the essential outline for the description of instantaneous bond structure. It is important to note that this virgin (undislocated) reference element, which shall henceforth be referred to as the *reference cell*, must thereafter be regarded as an integral part of any constitutive relation. It is also evident that in the absence of dislocations, specification of $\mathbf{F}_e$ would provide a complete description of the local bond structure, and therefore determine the instantaneous state. Generally, however, additional information describing the dislocation induced change in material properties is required. Since dislocation patterns tend to be structurally "irregular" and are fundamentally history dependent, they are probably best described in terms of state variables which are statistically related to the density and spatial geometry of the "important" types of dislocation distributions. Based on these considerations it is assumed that an "adequate" description of local bond distribution, and therefore of state, can be formulated in terms of the cell placement tensor $\mathbf{F}_e$ and a set of N additional tensor state variables $\boldsymbol{q} = \{\tilde{\mathbf{q}}_\alpha\}_{\alpha=1}^{N}$ of the Eulerian† type. The definition of specific state variables shall not be attempted here although a particular example based on the phenomenology of "dislocation strain" shall be discussed in the concluding section.

Before assessing the consequences of this assumption, it is necessary to account for any structural symmetry. Indeed, if the characteristic material lattice, as embodied in the chosen reference cell, is symmetric with respect to a group of orthogonal rotations $\mathcal{G}$, then the cell placement $\mathbf{F}_e$ is completely indistinguishable from $\mathbf{F}_e\mathbf{Q}$ for any $\mathbf{Q} \in \mathcal{G}$. To account for this, the set of all possible cell placements shall be partitioned into nonempty, maximal equivalence classes $\mathcal{F}_e$ characterized by the relation

$$\mathbf{F}_e^* \sim \mathbf{F}_e \text{ if and only if } \mathbf{F}_e^* = \mathbf{F}_e\mathbf{Q} \text{ for some } \mathbf{Q} \in \mathcal{G} \tag{3.1}$$

in terms of the orthogonal symmetry group $\mathcal{G}$ of the reference cell. Having thus removed any indeterminacy in the specification of cell placement, the fundamental state variable hypothesis may now be stated in terms of the *state descriptor pair*

$$\boldsymbol{S} = (\mathcal{F}_e, \boldsymbol{q}) \tag{3.2}$$

consisting of a group of indistinguishable cell placements and an N-tuple of dislocation state

† "Eulerian" is used to distinguish variables which are defined and interpreted in relation to the current element configuration.

variables.† Specifically, it is assumed that there exists a one-to-one correspondence between the accessible states Σ for a material element and the set of state descriptors $\boldsymbol{S}$ as expressed through the relationships

$$\begin{aligned} \Sigma_t &= \hat{\Sigma}[\boldsymbol{S}(t)], \\ \boldsymbol{S}(t) &= \hat{\boldsymbol{S}}(\Sigma_t). \end{aligned} \tag{3.3}$$

With reference to (2.4), the symbol $\mathrm{T}_{\mathbf{Q}}$ shall henceforth be more broadly interpreted as the "appropriate" tensor transformation operator associated with element reorientation by proper orthogonal $\mathbf{Q}$. Element reorientation is thus seen to effect the following changes:

$$\begin{aligned} &\boldsymbol{\sigma} \to \mathrm{T}_{\mathbf{Q}}\boldsymbol{\sigma} = \mathbf{Q}\boldsymbol{\sigma}\mathbf{Q}^T, \\ &\psi \to \mathrm{T}_{\mathbf{Q}}\psi = \psi, \\ &\mathbf{F}_e \to \mathrm{T}_{\mathbf{Q}}\mathbf{F}_e = \mathbf{Q}\mathbf{F}_e, \\ &\mathscr{F}_e \to \mathrm{T}_{\mathbf{Q}}\mathscr{F}_e = \{\mathbf{F}_e : \mathbf{Q}^T\mathbf{F}_e \in \mathscr{F}_e\}, \\ &\tilde{\mathbf{q}}_\alpha \to \mathrm{T}_{\mathbf{Q}}\tilde{\mathbf{q}}_\alpha; \qquad \alpha = 1, \ldots, N, \\ &\boldsymbol{q} \to \mathrm{T}_{\mathbf{Q}}\boldsymbol{q} = \{\mathrm{T}_{\mathbf{Q}}\tilde{\mathbf{q}}_\alpha\}_{\alpha=1}^{N}, \\ &\boldsymbol{R} \to \mathrm{T}_{\mathbf{Q}}\boldsymbol{R} = [\mathrm{T}_{\mathbf{Q}}\boldsymbol{\sigma}, \mathrm{T}_{\mathbf{Q}}\psi], \\ &\boldsymbol{S} \to \mathrm{T}_{\mathbf{Q}}\boldsymbol{S} = [\mathrm{T}_{\mathbf{Q}}\boldsymbol{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}]. \end{aligned} \tag{3.4}$$

With this and the definition of $T_{\mathbf{Q}}\Sigma$ it is clearly necessary to require that the functions in (3.3) satisfy

$$\begin{aligned} T_{\mathbf{Q}}[\hat{\Sigma}(\boldsymbol{S})] &= \hat{\Sigma}(\mathrm{T}_{\mathbf{Q}}\boldsymbol{S}), \\ \mathrm{T}_{\mathbf{Q}}\boldsymbol{S} &= \hat{\boldsymbol{S}}(T_{\mathbf{Q}}\Sigma), \end{aligned} \tag{3.5}$$

for all proper orthogonal $\mathbf{Q}$.

For materials having this sort of finite dimensional state space, the response and evolution functionals (2.7) can be recast in the form

$$\begin{aligned} \boldsymbol{R}(\tau) &= \mathscr{R}[\boldsymbol{S}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t], \\ \boldsymbol{S}(\tau) &= \mathscr{E}[\boldsymbol{S}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t]; \qquad \tau > t, \end{aligned} \tag{3.6}$$

expressed in terms of the state descriptor $\boldsymbol{S}$. With reference to (2.8, 10) and (3.5) it is clear that both of these functionals are subject to rotational invariance through

$$\mathscr{K}[\boldsymbol{S}, \mathbf{F}; \mathbf{C}] = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}\{\mathscr{K}[\boldsymbol{S}, \mathbf{QF}; \mathbf{C}]\} \\ \mathscr{K}[\mathrm{T}_{\mathbf{Q}}\boldsymbol{S}, \mathbf{FQ}^T; \mathbf{QCQ}^T] \end{cases} \tag{3.7}$$

for all proper orthogonal $\mathbf{Q}$, in addition to the consistency condition (2.9). With the introduction of the surjective mapping

$$\hat{\mathscr{F}}_e(\mathbf{F}_e) \equiv \{\mathbf{F}_e^* : \mathbf{F}_e^* = \mathbf{F}_e\mathbf{Q} \text{ for some } \mathbf{Q} \in \mathscr{G}\}, \tag{3.8}$$

which clearly satisfies

$$\mathrm{T}_{\mathbf{Q}}[\hat{\mathscr{F}}_e(\mathbf{F}_e)] = \hat{\mathscr{F}}_e(\mathbf{QF}_e), \tag{3.9}$$

† The current mass density ρ must be considered a primary quantity in the determination of state. If inelastic deformation is assumed to be isochoric (as it usually is), then $\rho = \rho_0/\det(\mathbf{F}_e)$, in terms of the reference cell mass density ρ_0. If this constraint is not imposed, then ρ should be regarded as a constituent of $\boldsymbol{q}$.

the respective domains of these functionals can be extended over the set of all possible cell placements. This leads to the functional forms

$$\begin{aligned} \boldsymbol{R}(\tau) &= [\mathbf{F}_e, \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t], \\ \mathscr{F}_e(\tau) &= \bar{\mathscr{E}}_e[\mathbf{F}_e, \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t], \\ \boldsymbol{q}(\tau) &= \mathscr{E}_q[\mathbf{F}_e, \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t]\,; \qquad \text{for any } \mathbf{F}_e \in \mathscr{F}_e(t) \text{ and } \tau > t, \end{aligned} \tag{3.10}$$

subject to consistency and rotational invariance through

$$\mathscr{H}[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}\{\mathscr{H}[\mathbf{F}_e, \boldsymbol{q}, \mathbf{QF}\,;\, \mathbf{C}]\} \\ \mathscr{H}[\mathbf{QF}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{FQ}^T\,;\, \mathbf{QCQ}^T]\,; \quad \text{for all proper orthogonal } \mathbf{Q}. \end{cases} \tag{3.11}$$

In view of the functional independence on $\mathbf{F}_e$ within each respective equivalence class $\mathscr{F}_e$ it would clearly suffice to replace $(3.10)_2$ with a more specific evolution function of the form

$$\mathbf{F}_e(\tau) = \mathscr{E}_e[\mathbf{F}_e, \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t]\,; \qquad \text{for each } \mathbf{F}_e \in \mathscr{F}_e(t) \text{ and } \tau > t, \tag{3.12}$$

provided only that the relation

$$\mathscr{E}_e[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] \in \bar{\mathscr{E}}_e[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] \tag{3.13}$$

is always satisfied. It must be emphasized that there would exist a multiplicity of acceptable functionals for any material having a nontrivial symmetry group $\mathscr{G}$. A particularly direct method for selecting such a functional is to choose a representative, or "distinguished", element from each equivalence class $\mathscr{F}_e$, and thereby establish a one-to-one correspondence

$$\mathbf{F}_e^* = \pi(\mathscr{F}_e)\,; \qquad \mathscr{F}_e = \pi^{-1}(\mathbf{F}_e^*) \tag{3.14}$$

between the set of $\mathbf{F}_e$-equivalence classes and the subset of distinguished cell placement tensors. A functional $\mathscr{E}_e$ can then be defined on the set of distinguished element placements through functional composition, i.e.

$$\begin{aligned} \mathbf{F}_e^*(\tau) &= \mathscr{E}_e[\mathbf{F}_e^*(t), \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t] \\ &\equiv (\pi \circ \bar{\mathscr{E}}_e)[\mathbf{F}_e^*(t), \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t]. \end{aligned} \tag{3.15}$$

The domain and range of $\mathscr{E}_e$ can then be extended, consistent with (3.13), to the full range of cell placements by stipulating that

$$\mathscr{E}_e[\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] = \{\mathscr{E}_e[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}]\}\mathbf{Q}\,; \qquad \text{for each } \mathbf{Q} \in \mathscr{G}. \tag{3.16}$$

In this manner an acceptable (but generally nonunique) evolution form

$$\mathbf{F}_e(\tau) = \mathscr{E}_e[\mathbf{F}_e(t), \boldsymbol{q}(t), \mathbf{F}(\tau)\,;\, \mathbf{C}_\tau^t], \tag{3.17}$$

satisfying

$$\mathscr{E}_e[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] = \{\mathscr{E}_e[\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}]\}\mathbf{Q}^T, \qquad \text{for each } \mathbf{Q} \in \mathscr{G}, \tag{3.18}$$

can be generated. It is a simple matter to confirm that

$$\bar{\mathscr{E}}_e[\mathbf{F}_e, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}] \equiv \mathscr{E}_e[\mathbf{F}_e\mathbf{Q}_1, \boldsymbol{q}, \mathbf{F}\,;\, \mathbf{C}]\mathbf{Q}_2^T, \tag{3.19}$$

for any pair $(\mathbf{Q}_1, \mathbf{Q}_2) \subseteq \mathscr{G}$, also defines an acceptable evolution form.

These considerations lead to the proposal of a state variable format for the constitutive modeling of inelastic solids based on response and evolution functionals having the form

$$\begin{aligned} \boldsymbol{R}(\tau) &= [\sigma(\tau), \psi(\tau)] = \mathscr{R}[\mathbf{F}_e(t)\mathbf{Q}, \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t], \\ \mathbf{F}_e(\tau) &= \mathscr{E}_e[\mathbf{F}_e(t)\mathbf{Q}, \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t]\mathbf{Q}^T, \\ \boldsymbol{q}(\tau) &= \{\tilde{\mathbf{q}}_\alpha(\tau)\}_{\alpha=1}^N = \mathscr{E}_q[\mathbf{F}_e(t)\mathbf{Q}, \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t]; \qquad \text{for each } \mathbf{Q} \in \mathscr{G} \text{ and } \tau > t. \end{aligned} \tag{3.20}$$

Each of these functionals is subject to the consistency condition as expressed through (2.9), and rotational invariance through (3.11).

A particularly important special case is for fully isotropic cell structure and a full proper orthogonal symmetry group $\mathscr{G} = \Theta$. This will most likely occur with polycrystalline aggregate for which a characteristic cell consists of a large number of randomly oriented grains. By making use of the polar decomposition theorem, $\mathbf{F}_e$ can be written in the form

$$\mathbf{F}_e = \mathbf{b}^{1/2}\mathbf{R}_e, \tag{3.21}$$

in terms of an orthogonal elastic rotation tensor $\mathbf{R}_e$ and a symmetric elastic deformation tensor

$$\mathbf{b} \equiv \mathbf{F}_e\mathbf{F}_e^T. \tag{3.22}$$

Since

$$\mathbf{b}^{1/2} = \sqrt{\mathbf{F}_e\mathbf{F}_e^T} \in \hat{\mathscr{F}}_e(\mathbf{F}_e); \qquad \text{for all } \mathbf{F}_e, \tag{3.23}$$

this stretch entry may be selected as the distinguished element from each $\mathbf{F}_e$-equivalence class. For this choice in (3.15) and the substitution of $\mathbf{Q} = \mathbf{R}_e^T$ in (3.20), the structurally isotropic forms are obtained, viz.

$$\begin{aligned} \boldsymbol{R}(\tau) &= \mathscr{R}[\mathbf{b}^{1/2}(t), \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t], \\ \mathbf{b}^{1/2}(\tau) &= \mathscr{E}_e[\mathbf{b}^{1/2}(t), \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t], \\ \boldsymbol{q}(\tau) &= \mathscr{E}_q[\mathbf{b}^{1/2}(t), \boldsymbol{q}(t), \mathbf{F}(\tau); \mathbf{C}_\tau^t]; \qquad \tau > t. \end{aligned} \tag{3.24}$$

In view of (3.23) these equations are automatically invariant with respect to reference cell rotation although they are still subject to consistency and rotational invariance through

$$\mathscr{H}[\mathbf{b}^{1/2}, \boldsymbol{q}, \mathbf{F}; \mathbf{C}] = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}\{\mathscr{H}[\mathbf{b}^{1/2}, \boldsymbol{q}, \mathbf{QF}; \mathbf{C}]\} \\ \mathscr{H}[\mathrm{T}_{\mathbf{Q}}\mathbf{b}^{1/2}, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{FQ}^T; \mathbf{QCQ}^T], \end{cases} \tag{3.25}$$

where

$$\mathrm{T}_{\mathbf{Q}}\mathbf{b}^{1/2} = \mathbf{Q}\mathbf{b}^{1/2}\mathbf{Q}^T, \tag{3.26}$$

for all proper orthogonal $\mathbf{Q}$. It is also evident that these forms could readily be replaced with equivalent ones expressed in terms of either of the symmetric cell deformation tensors $\mathbf{b}$, $\mathbf{c} = \mathbf{b}^{-1}$, or any other cell strain measure

$$\mathbf{e} = \hat{\mathbf{e}}(\mathbf{b}) \tag{3.27}$$

defined through an invertible isotropic tensor mapping $\hat{\mathbf{e}}$.

B. *Reduced forms*

The imposition of additional smoothness assumptions makes it possible to replace these causal functional relationships with simpler and more familiar response functions and differential, or rate type, state evolution equations. To illustrate, suppose that one wishes to model a material which exhibits initial, rate-independent, elastic response to a suddenly applied load. For such a material it would seem appropriate to assume that any continuous stimulus (deformation process) elicits a continuous response. In view of (2.23), it is then possible to replace $(3.20)_1$ with the response form

$$\boldsymbol{R}(t) = [\sigma(t), \psi(t)] = \hat{\boldsymbol{R}}[\mathbf{F}_e(t), \boldsymbol{q}(t)] \tag{3.28}$$

subject to rotational invariance through

$$\hat{\boldsymbol{R}}(\mathbf{F}_e, \boldsymbol{q}) = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}[\hat{\boldsymbol{R}}(\mathbf{Q}\mathbf{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q})]; & \text{for each } \mathbf{Q} \in \Theta, \\ \hat{\boldsymbol{R}}(\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}); & \text{for each } \mathbf{Q} \in \mathscr{G}, \end{cases} \tag{3.29}$$

in terms of the full proper orthogonal group Θ. Similarly, if the initial response of a material is similar to that of a Kelvin–Voigt-type viscoelastic solid, it might then seem more appropriate to assume that smooth stimuli are required to elicit continuous response. This would give rise to the response form

$$\boldsymbol{R}(t) = [\sigma(t), \psi(t)] = \hat{\boldsymbol{R}}[\mathbf{F}_e(t), \boldsymbol{q}(t), \mathbf{D}(t)] \tag{3.30}$$

subject to

$$\hat{\boldsymbol{R}}(\mathbf{F}_e, \boldsymbol{q}, \mathbf{D}) = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}[\hat{\boldsymbol{R}}(\mathbf{Q}\mathbf{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{Q}\mathbf{D}\mathbf{Q}^T)]; & \text{for each } \mathbf{Q} \in \Theta, \\ \hat{\boldsymbol{R}}(\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{D}); & \text{for each } \mathbf{Q} \in \mathscr{G}. \end{cases} \tag{3.31}$$

The generalized response forms which apply to materials which respond continuously to C_K stimuli, in terms of the state descriptors and the first K Rivlin–Ericksen tensors, is immediately evident.

The evolution functionals $(3.20)_2$ and $(3.20)_3$ may be reduced in similar manner through (2.24, 25). In particular, if it is assumed that the state descriptors evolve smoothly (C_1) during sufficiently smooth (C_K) deformations, then, at each instant during such a deformation process,

$$\begin{aligned} \mathring{\mathbf{F}}_e &= \dot{\mathbf{F}}_e - \mathbf{W}\mathbf{F}_e = \boldsymbol{\mu}_e(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \\ \mathring{\mathbf{q}}_\alpha &= \tilde{\boldsymbol{\mu}}_\alpha(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K); \qquad \alpha = 1, \ldots, N, \end{aligned} \tag{3.32}$$

subject to

$$\boldsymbol{\mu}_e(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K) = \begin{cases} \mathbf{Q}^T[\boldsymbol{\mu}_e(\mathbf{Q}\mathbf{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{Q}\mathbf{A}_1\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K\mathbf{Q}^T)]; & \text{for each } \mathbf{Q} \in \Theta, \\ [\boldsymbol{\mu}_e(\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K)]\mathbf{Q}^T; & \text{for each } \mathbf{Q} \in \mathscr{G}, \end{cases} \tag{3.33}$$

$$\boldsymbol{\mu}_\alpha(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K) = \begin{cases} \mathrm{T}_{\mathbf{Q}^T}[\tilde{\boldsymbol{\mu}}_\alpha(\mathbf{Q}\mathbf{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{Q}\mathbf{A}_1\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K\mathbf{Q}^T)]; & \text{for each } \mathbf{Q} \in \Theta, \\ \tilde{\boldsymbol{\mu}}_\alpha(\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K); & \text{for each } \mathbf{Q} \in \mathscr{G}. \end{cases} \tag{3.34}$$

With reference to the fully isotropic functional forms (3.24, 25, 26) it is clear that smoothness assumptions of this type give rise to the structurally isotropic response and

evolution forms

$$\begin{aligned} \boldsymbol{R} &= [\sigma, \psi] = \hat{\boldsymbol{R}}(\mathbf{e}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \\ \mathring{\mathbf{e}} &= \boldsymbol{v}_e(\mathbf{e}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \\ \mathring{\mathbf{q}}_\alpha &= \boldsymbol{v}_\alpha(\mathbf{e}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K); \qquad \alpha = 1, \ldots, N, \end{aligned} \tag{3.35}$$

in terms of a finite number of Rivlin–Ericksen tensors and any elastic strain measure $\mathbf{e}$ defined through an invertible, isotropic tensor function of $\mathbf{b} = \mathbf{F}_e\mathbf{F}_e^T$. These functions are constrained by rotational invariance through

$$\mathrm{T}_\mathbf{Q}[h(\mathbf{e}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K)] = h(\mathrm{T}_\mathbf{Q}\mathbf{e}, \mathrm{T}_\mathbf{Q}\boldsymbol{q}, \mathbf{Q}\mathbf{A}_1\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K\mathbf{Q}^T); \qquad \text{for each } \mathbf{Q} \in \Theta, \tag{3.36}$$

with

$$\mathrm{T}_\mathbf{Q}\mathbf{e} = \mathbf{Q}\mathbf{e}\mathbf{Q}^T \to \mathring{\mathbf{e}} = \dot{\mathbf{e}} + \mathbf{e}\mathbf{W} - \mathbf{W}\mathbf{e}. \tag{3.37}$$

Based on these considerations it is evident that "smooth" response and evolution functionals give way to response functions and incremental rate equations for the relevant state variables. These rate equations, by virtue of the existence and uniqueness of solutions to systems of first-order, ordinary differential equations, "assign" to each sufficiently smooth stimulus, $\mathbf{F}_\tau^t$, a smooth trajectory, $\boldsymbol{S}_\tau^t$, in the finite dimensional state descriptor space subject to admissible initial conditions $\boldsymbol{S}(t) = \boldsymbol{S}_t$. It is important to note that while the functions (as opposed to functionals) appearing in these equations are still subject to the rotational invariance requirements associated with objectivity and reference cell isotropy, the forms themselves are inherently consistent in the sense of (2.9). Also, if piecewise smooth stimuli are to be allowed, then these evolution equations must be supplemented with "jump" conditions which determine the change of state at a stimulus singularity.

C. *Elastic rate forms*

Relating to this latter point is the fact that a purely elastic deformation $\mathbf{F}$ elicits the following changes in the elastic descriptors $\mathbf{F}_e$, $\mathbf{b} = \mathbf{F}_e\mathbf{F}_e^T$ and $\mathbf{c} = \mathbf{b}^{-1}$:

$$\begin{aligned} &\mathbf{F}_e \to \mathbf{F}\mathbf{F}_e, \\ &\mathbf{b} \to \mathbf{F}\mathbf{b}\mathbf{F}^T, \\ &\mathbf{c} \to (\mathbf{F}^{-1})^T\mathbf{c}(\mathbf{F}^{-1}). \end{aligned} \tag{3.38}$$

These evolution forms apply to an instantaneous elastic deformation as well as to one which proceeds smoothly. For smooth elastic deformations, it is easily seen that these elastic descriptors evolve according to the rate forms

$$\begin{aligned} &\dot{\mathbf{F}}_e = \mathbf{L}\mathbf{F}_e, \\ &\dot{\mathbf{b}} = \mathbf{L}\mathbf{b} + \mathbf{b}\mathbf{L}^T, \\ &\dot{\mathbf{c}} = -(\mathbf{c}\mathbf{L} + \mathbf{L}^T\mathbf{c}). \end{aligned} \tag{3.39}$$

With reference to the general rate forms $(3.32)_1$, $(3.35)_2$ and (3.37), it is a simple exercise to establish that they may be recast in the equivalent forms:

$$\begin{aligned} \dot{\mathbf{F}}_e = \mathbf{L}\mathbf{F}_e - \mathbf{F}_e\boldsymbol{\Lambda} \to \mathbf{F}_e\boldsymbol{\Lambda} &= \mathbf{D}\mathbf{F}_e - \boldsymbol{\mu}_e, \\ \dot{\mathbf{b}} = \mathbf{L}\mathbf{b} + \mathbf{b}\mathbf{L}^T + 2\boldsymbol{\Gamma}_b \to 2\boldsymbol{\Gamma}_b &= \boldsymbol{v}_b - (\mathbf{b}\mathbf{D} + \mathbf{D}\mathbf{b}), \\ \dot{\mathbf{c}} = -(\mathbf{c}\mathbf{L} + \mathbf{L}^T\mathbf{c}) + 2\boldsymbol{\Gamma}_c \to 2\boldsymbol{\Gamma}_c &= \boldsymbol{v}_c + (\mathbf{c}\mathbf{D} + \mathbf{D}\mathbf{c}), \end{aligned} \tag{3.40}$$

expressed in terms of the inelastic "velocity gradient"

$$\mathbf{\Lambda} = \hat{\mathbf{\Lambda}}(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \tag{3.41}$$

subject to rotational invariance through

$$\hat{\mathbf{\Lambda}}(\mathbf{F}_e, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K) = \begin{cases} \hat{\mathbf{\Lambda}}(\mathbf{Q}\mathbf{F}_e, \mathrm{T}_{\mathbf{Q}}\boldsymbol{q}, \mathbf{Q}\mathbf{A}_1\mathbf{Q}^T, \ldots, \mathbf{Q}\mathbf{A}_K\mathbf{Q}^T); & \text{for each } \mathbf{Q} \in \Theta, \\ \mathbf{Q}\hat{\mathbf{\Lambda}}(\mathbf{F}_e\mathbf{Q}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K)\mathbf{Q}^T; & \text{for each } \mathbf{Q} \in \mathscr{G}, \end{cases} \tag{3.42}$$

and symmetric "slippage" tensors

$$\begin{aligned} \mathbf{\Gamma}_b &= \hat{\mathbf{\Gamma}}_b(\mathbf{b}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \\ \mathbf{\Gamma}_c &= \hat{\mathbf{\Gamma}}_c(\mathbf{c}, \boldsymbol{q}, \mathbf{A}_1, \ldots, \mathbf{A}_K), \end{aligned} \tag{3.43}$$

subject to (3.36).

In order to choose specific forms for these inelastic rate terms it is essential to understand their physical significance. This is easily accomplished by considering the relationships

$$\mathbf{x} = \mathbf{F}_e \cdot \mathbf{X}; \qquad \mathbf{X} = \mathbf{F}_e^{-1} \cdot \mathbf{x} \tag{3.44}$$

between material directors $\mathbf{x}$ in the current configuration and their lattice director counterparts $\mathbf{X}$ in the reference cell. By letting $\mathbf{x} = \mathbf{x}(t)$ represent a fixed material director, so that $\dot{\mathbf{x}} = \mathbf{L} \cdot \mathbf{x}$, and $\mathbf{X} = \mathbf{X}(t) = \mathbf{F}_e^{-1}(t) \cdot \mathbf{x}(t)$ its time dependent reference cell "image", it is easily confirmed that

$$\begin{aligned} \dot{\mathbf{x}} &= \dot{\mathbf{F}}_e \cdot \mathbf{X} + \mathbf{F}_e \cdot \dot{\mathbf{X}}, \\ \mathbf{L} \cdot \mathbf{x} &= (\mathbf{L}\mathbf{F}_e - \mathbf{F}_e\mathbf{\Lambda}) \cdot \mathbf{X} + \mathbf{F}_e \cdot \dot{\mathbf{X}}, \\ \mathbf{L} \cdot \mathbf{x} &= \mathbf{L} \cdot \mathbf{x} + \mathbf{F}_e \cdot (\dot{\mathbf{X}} - \mathbf{\Lambda} \cdot \mathbf{X}) \rightarrow \dot{\mathbf{X}} = \mathbf{\Lambda} \cdot \mathbf{X}. \end{aligned} \tag{3.45}$$

Thus, the inelastic rate $\mathbf{\Lambda}$ is seen to represent the velocity gradient associated with the material flow in the reference cell.

The relation

$$\mathbf{X}_1 \cdot \mathbf{X}_2 = \mathbf{x}_1 \cdot \mathbf{c} \cdot \mathbf{x}_2 \tag{3.46}$$

serves to establish $\mathbf{c} = \mathbf{b}^{-1}$ as the deformation, or "metric" tensor which relates the current and "relaxed" element geometries. By letting $\mathbf{x}_1 = \mathbf{x}_1(t)$ and $\mathbf{x}_2 = \mathbf{x}_2(t)$ represent a pair of fixed (flow embedded) material directors, with $\mathbf{X}_1 = \mathbf{F}_e^{-1} \cdot \mathbf{x}_1$ and $\mathbf{X}_2 = \mathbf{F}_e^{-1} \cdot \mathbf{x}_2$ as before, it follows that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{X}_1 \cdot \mathbf{X}_2) &= \mathbf{x}_1 \cdot \dot{\mathbf{c}} \cdot \mathbf{x}_2 + \dot{\mathbf{x}}_1 \cdot \mathbf{c} \cdot \mathbf{x}_2 + \mathbf{x}_1 \cdot \mathbf{c} \cdot \dot{\mathbf{x}}_2 \\ &= \mathbf{x}_1 \cdot [\dot{\mathbf{c}} + \mathbf{L}^T\mathbf{c} + \mathbf{c}\mathbf{L}] \cdot \mathbf{x}_2 \\ &= \mathbf{x}_1 \cdot 2\mathbf{\Gamma}_c \cdot \mathbf{x}_2. \end{aligned} \tag{3.47}$$

Comparison of this with the expression

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{X}_1 \cdot \mathbf{X}_2) = \mathbf{X}_1 \cdot 2\mathbf{\Lambda}_s \cdot \mathbf{X}_2, \tag{3.48}$$

in terms of the symmetric rate of deformation tensor $\mathbf{\Lambda}_s \equiv \mathrm{sym}(\mathbf{\Lambda})$ associated with the

material flow in the reference cell, leads to the correspondence

$$\Gamma_c = (\mathbf{F}_e^{-1})^T \mathbf{A}_s (\mathbf{F}_e^{-1}). \tag{3.49}$$

In view of the identity $\Gamma_b = -\mathbf{b}\Gamma_c\mathbf{b}$ ($\dot{\mathbf{b}} = -\mathbf{b}\dot{\mathbf{c}}\mathbf{b}$), it also follows that

$$\Gamma_b = -\mathbf{F}_e \mathbf{A}_s \mathbf{F}_e^T. \tag{3.50}$$

Particularly convenient alternative forms for the evolution equations $(3.40)_2$ and $(3.40)_3$ are

$$\begin{aligned} \mathring{\mathbf{b}} &= \dot{\mathbf{b}} + \mathbf{b}\mathbf{W} - \mathbf{W}\mathbf{b} = \mathbf{b}(\mathbf{D}-\mathbf{d}) + (\mathbf{D}-\mathbf{d})\mathbf{b}, \\ \mathring{\mathbf{c}} &= \dot{\mathbf{c}} + \mathbf{c}\mathbf{W} - \mathbf{W}\mathbf{c} = \mathbf{c}(\mathbf{d}-\mathbf{D}) + (\mathbf{d}-\mathbf{D})\mathbf{c}, \end{aligned} \tag{3.51}$$

expressed in terms of the symmetric inelastic rate $\mathbf{d}$ which is defined as the unique (symmetric) solution to

$$\mathbf{c}\mathbf{d} + \mathbf{d}\mathbf{c} = 2\Gamma_c. \tag{3.52}$$

4. SOME USEFUL MODELS

A. *Elasticity*

In order to demonstrate the scope and utility of this format a number of examples shall now be considered. It should be noted that these examples encompass virtually all successful three-dimensional models currently in use.

The simplest model is that corresponding to a hyperelastic solid. In this model state is determined by reference cell placement, continuous stimuli (from the class of piecewise continuous stimuli) elicit continuous response, and the reference cell is "materially fixed" in the sense that it deforms with the material. In view of (3.28) and the elastic evolution forms (3.38, 39) the hyperelastic model takes the form

$$\begin{aligned} \psi &= \hat{\psi}(\mathbf{F}_e), \\ \boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}_e), \\ \dot{\mathbf{F}}_e &= \mathbf{L}\mathbf{F}_e, \\ (\mathbf{F}_e)_2 &= \mathbf{F}_{2/1}(\mathbf{F}_e)_1, \end{aligned} \tag{4.1}$$

subject to frame invariance through

$$\begin{aligned} &\hat{\psi}(\mathbf{F}_e) = \hat{\psi}(\mathbf{Q}\mathbf{F}_e), \\ &\hat{\boldsymbol{\sigma}}(\mathbf{F}_e) = \mathbf{Q}^T \hat{\boldsymbol{\sigma}}(\mathbf{Q}\mathbf{F}_e)\mathbf{Q}; \qquad \text{for each } \mathbf{Q} \in \Theta, \end{aligned} \tag{4.2}$$

and material symmetry through

$$\begin{aligned} &\hat{\psi}(\mathbf{F}_e) = \hat{\psi}(\mathbf{F}_e\mathbf{Q}), \\ &\hat{\boldsymbol{\sigma}}(\mathbf{F}_e) = \hat{\boldsymbol{\sigma}}(\mathbf{F}_e\mathbf{Q}); \qquad \text{for each } \mathbf{Q} \in \mathcal{G}. \end{aligned} \tag{4.3}$$

The invariance condition $(4.2)_1$ makes it possible to recast the energy equation in the form

$$\psi = \bar{\psi}(\mathbf{C}_e); \qquad \mathbf{C}_e \equiv \mathbf{F}_e^T \mathbf{F}_e, \tag{4.4}$$

subject only to the material symmetry condition

$$\bar{\psi}(\mathbf{C}_e) = \bar{\psi}(\mathbf{Q}^T \mathbf{C}_e \mathbf{Q}); \qquad \text{for each } \mathbf{Q} \in \mathcal{G}. \tag{4.5}$$

After noting that

$$\begin{aligned} \dot{\mathbf{C}}_e &= \mathbf{F}_e^T 2\mathbf{D}\mathbf{F}_e, \\ (\mathbf{C}_e)_2 &= (\mathbf{F}_e)_1^T \mathbf{C}_{2/1} (\mathbf{F}_e)_1; \qquad \mathbf{C}_{2/1} \equiv \mathbf{F}_{2/1}^T \mathbf{F}_{2/1}, \end{aligned} \tag{4.6}$$

the Clausius–Duhem (dissipation) inequality

$$\boldsymbol{\sigma} \cdot \mathbf{D} - \rho \dot{\psi} \geqslant 0 \tag{4.7}$$

may be expanded to obtain

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{D} - \rho \frac{\partial \psi}{\partial \mathbf{C}_e} \cdot \dot{\mathbf{C}}_e &\geqslant 0, \\ \boldsymbol{\sigma} \cdot \mathbf{D} - \rho_0 \det{}^{-1}(\mathbf{F}_e) \frac{\partial \psi}{\partial \mathbf{C}_e} \cdot (\mathbf{F}_e^T 2\mathbf{D}\mathbf{F}_e) &\geqslant 0, \\ \left\{ \boldsymbol{\sigma} - 2\rho_0 \det{}^{-1}(\mathbf{F}_e) \left[\mathbf{F}_e \frac{\partial \psi}{\partial \mathbf{C}_e} \mathbf{F}_e^T \right] \right\} \cdot \mathbf{D} &\geqslant 0, \end{aligned} \tag{4.8}$$

in terms of the reference cell mass density ρ_0. Thus, it is necessary to require that

$$\boldsymbol{\sigma} = 2\rho_0 \det{}^{-1}(\mathbf{F}_e) \left[\mathbf{F}_e \frac{\partial \psi}{\partial \mathbf{C}_e} \mathbf{F}_e^T \right]. \tag{4.9}$$

It is customary to introduce the symmetric Piola–Kirchhoff stress

$$\mathbf{S} = \hat{\mathbf{S}}(\mathbf{C}_e) \equiv 2\rho_0 \frac{\partial \psi}{\partial \mathbf{C}_e} = \rho_0 \frac{\partial \psi}{\partial \mathbf{E}_e}; \qquad 2\mathbf{E}_e \equiv \mathbf{C}_e - \mathbf{I} \tag{4.10}$$

which, in turn, determines the Cauchy stress through the expression

$$\boldsymbol{\sigma} = \det{}^{-1}(\mathbf{F}_e) \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T. \tag{4.11}$$

It is a simple matter to confirm that this stress response equation automatically satisfies $(4.2)_2$ and $(4.3)_2$ by virtue of the fact that

$$\hat{\mathbf{S}}(\mathbf{C}_e) = \mathbf{Q} \hat{\mathbf{S}}(\mathbf{Q}^T \mathbf{C}_e \mathbf{Q}) \mathbf{Q}^T; \qquad \text{for each } \mathbf{Q} \in \mathcal{G}, \tag{4.12}$$

which follows as a consequence of (4.5). In addition, if all deformations are measured from a particular unstressed reference configuration for which $\mathbf{F}_e = (\mathbf{F}_e)_0 = \mathbf{I}$, then $\mathbf{F}_e$ may be interpreted as the full deformation gradient $\mathbf{F}$, and $\mathbf{C}_e$ as the left Cauchy–Green tensor.

For the fully isotropic case ($\mathcal{G} = \Theta$),

$$\psi = \bar{\psi}(\mathbf{C}_e) = \bar{\psi}(\mathbf{Q}^T \mathbf{C}_e \mathbf{Q}); \qquad \text{for each } \mathbf{Q} \in \Theta, \tag{4.13}$$

it must necessarily follow that

$$\psi = \bar{\psi}(\mathbf{C}_e) = \tilde{\psi}(\mathrm{I}_{C_e}, \mathrm{II}_{C_e}, \mathrm{III}_{C_e}) \tag{4.14}$$

in terms of the principal invariants of $\mathbf{C}_e$. Since the principal invariants of $\mathbf{b} = \mathbf{F}_e \mathbf{F}_e^T$ are identical to those of $\mathbf{C}_e$ it follows that

$$\bar{\psi}(\mathbf{C}_e) = \bar{\psi}(\mathbf{b}). \tag{4.15}$$

Moreover,

$$\mathbf{S} = \hat{\mathbf{S}}(\mathbf{C}_e) = 2\rho_0 \frac{\partial \psi}{\partial \mathbf{C}_e} = \alpha \mathbf{I} + \beta \mathbf{C}_e + \gamma \mathbf{C}_e^2 \tag{4.16}$$

in terms of scalar functions α, β and γ of the $\mathbf{C}_e$ (or $\mathbf{b}$) invariants, and hence

$$\begin{aligned} \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T &= \alpha \mathbf{b} + \beta \mathbf{b}^2 + \gamma \mathbf{b}^3 \\ &= [\alpha \mathbf{I} + \beta \mathbf{b} + \gamma \mathbf{b}^2]\mathbf{b} \\ &= \hat{\mathbf{S}}(\mathbf{b})\mathbf{b} \\ \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T &= 2\rho_0 \frac{\partial \psi}{\partial \mathbf{b}} \mathbf{b}. \end{aligned} \tag{4.17}$$

Since

$$\rho = \rho_0 / \det(\mathbf{F}_e) = \rho_0 / \sqrt{\det(\mathbf{b})}, \tag{4.18}$$

it therefore follows, via (4.11), that isotropic hyperelastic materials are represented by equations of the form

$$\begin{gathered} \psi = \bar{\psi}(\mathbf{b}) = \tilde{\psi}(\mathrm{I}_\mathbf{b}, \mathrm{II}_\mathbf{b}, \mathrm{III}_\mathbf{b}), \qquad \boldsymbol{\sigma} = 2\rho \frac{\partial \psi}{\partial \mathbf{b}} \mathbf{b}; \qquad \rho = \rho_0 / \sqrt{\det(\mathbf{b})}, \\ \dot{\mathbf{b}} = \mathbf{L}\mathbf{b} + \mathbf{b}\mathbf{L}^T, \qquad \mathbf{b}_2 = \mathbf{F}_{2/1} \mathbf{b}_1 \mathbf{F}_{2/1}^T. \end{gathered} \tag{4.19}$$

With reference to (3.35, 36), a more direct derivation of these isotropic forms begins with the fully isotropic response forms

$$\begin{aligned} \psi &= \hat{\psi}(\mathbf{b}), \\ \boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{b}) \end{aligned} \tag{4.20}$$

with the elastic evolution form $(3.39)_2$, subject to frame invariance through

$$\begin{aligned} \hat{\psi}(\mathbf{b}) &= \hat{\psi}(\mathbf{Q}\mathbf{b}\mathbf{Q}^T) \\ \hat{\boldsymbol{\sigma}}(\mathbf{b}) &= \mathbf{Q}^T \boldsymbol{\sigma}(\mathbf{Q}\mathbf{b}\mathbf{Q}^T)\mathbf{Q}; \qquad \text{for each } \mathbf{Q} \in \Theta. \end{aligned} \tag{4.21}$$

Due to the symmetry of $[(\partial \psi / \partial \mathbf{b})\mathbf{b}]$, substitution into the dissipation inequality (4.7) readily confirms the response form in (4.19).

The constitutive forms which apply to "small strain on large" are based on the approximation $\mathbf{L}\Delta t = (\nabla \mathbf{v})\nabla t \simeq \nabla \mathbf{u}$ in terms of the "small" displacement field $\mathbf{u}$ measured from the present strained configuration. With this, the rate expressions $(4.1)_3$, $(4.6)_1$, $(4.19)_3$, and the identity $\det(\mathbf{A})(\mathbf{A}^{-1})^T = \partial[\det(\mathbf{A})]/\partial \mathbf{A}$, it follows that a small deformation from a configuration having state $\mathbf{F}_e$ induces the approximate changes

$$\begin{aligned} \Delta \mathbf{F}_e &\simeq (\nabla \mathbf{u})\mathbf{F}_e, \\ \Delta[\det(\mathbf{F}_e)] &\simeq \det(\mathbf{F}_e) \cdot \mathrm{tr}(\boldsymbol{\varepsilon}), \\ \Delta \mathbf{C}_e &\simeq \mathbf{F}_e^T 2\boldsymbol{\varepsilon} \mathbf{F}_e, \\ \Delta \mathbf{b} &\simeq (\nabla \mathbf{u})\mathbf{b} + \mathbf{b}(\nabla \mathbf{u})^T, \end{aligned} \tag{4.22}$$

in terms of the small strain tensor

$$\boldsymbol{\varepsilon} \equiv \mathrm{sym}(\nabla \mathbf{u}) = \tfrac{1}{2}[(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T]. \tag{4.23}$$

Expansion of the stress response forms (4.9) and $(4.19)_2$ then leads to the regular and isotropic extra stress expressions

$$\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}(\nabla\mathbf{u})^T + (\nabla\mathbf{u})\boldsymbol{\sigma} - \boldsymbol{\sigma}\,\mathrm{tr}(\boldsymbol{\varepsilon}) + 2\rho\mathbf{F}_e\left[\left(\frac{\partial^2\psi}{\partial\mathbf{C}_e\otimes\partial\mathbf{C}_e}\right)\cdot(\mathbf{F}_e^T 2\boldsymbol{\varepsilon}\mathbf{F}_e)\right]\mathbf{F}_e^T,$$
$$\Delta\boldsymbol{\sigma} = (\nabla\mathbf{u})_A\boldsymbol{\sigma} - \boldsymbol{\sigma}(\nabla\mathbf{u})_A + [\partial\boldsymbol{\sigma}/\partial\mathbf{b}]\cdot(\mathbf{b}\boldsymbol{\varepsilon}+\boldsymbol{\varepsilon}\mathbf{b}). \tag{4.24}$$

A Kelvin–Voigt viscoelastic model would make use of the same state space and state evolution forms but would be assumed to respond continuously only to smooth (C_1) stimuli (from the class of allowable, continuous, piecewise smooth stimuli). With reference to (3.30,31), this model takes the form

$$\begin{aligned}\psi &= \hat{\psi}(\mathbf{F}_e, \mathbf{D}),\\ \boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}_e, \mathbf{D}),\\ \dot{\mathbf{F}}_e &= \mathbf{L}\mathbf{F}_e,\\ (\mathbf{F}_e)_2 &= \mathbf{F}_{2/1}(\mathbf{F}_e)_1,\end{aligned} \tag{4.25}$$

subject to

$$\hat{\psi}(\mathbf{F}_e, \mathbf{D}) = \begin{cases}\hat{\psi}(\mathbf{Q}\mathbf{F}_e, \mathbf{Q}\mathbf{D}\mathbf{Q}^T); & \text{for each } \mathbf{Q}\in\Theta,\\ \hat{\psi}(\mathbf{F}_e\mathbf{Q}, \mathbf{D}); & \text{for each } \mathbf{Q}\in\mathcal{G},\end{cases}$$

and (4.26)

$$\hat{\boldsymbol{\sigma}}(\mathbf{F}_e, \mathbf{D}) = \begin{cases}\mathbf{Q}^T\hat{\boldsymbol{\sigma}}(\mathbf{Q}\mathbf{F}_e, \mathbf{Q}\mathbf{D}\mathbf{Q}^T)\mathbf{Q}; & \text{for each } \mathbf{Q}\in\Theta,\\ \hat{\boldsymbol{\sigma}}(\mathbf{F}_e\mathbf{Q}, \mathbf{D}); & \text{for each } \mathbf{Q}\in\mathcal{G}.\end{cases}$$

After expanding the dissipation inequality (4.7) and noting that $\dot{\mathbf{D}}$ may be selected arbitrarily as one proceeds from a given state (piecewise smooth stimuli), it necessarily follows that

$$\frac{\partial\psi}{\partial\mathbf{D}} = 0 \rightarrow \psi = \hat{\psi}(\mathbf{F}_e) = \bar{\psi}(\mathbf{C}_e) \tag{4.27}$$

subject to (4.5), and

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}_f\begin{cases}\boldsymbol{\sigma}_e = 2\rho_0\det^{-1}(\mathbf{F}_e)\mathbf{F}_e\dfrac{\partial\psi}{\partial\mathbf{C}_e}\mathbf{F}_e^T,\\ \boldsymbol{\sigma}_f = \hat{\boldsymbol{\sigma}}_f(\mathbf{F}_e, \mathbf{D}),\end{cases} \tag{4.28}$$

with the choice of $\boldsymbol{\sigma}_f$ subject to

$$\boldsymbol{\sigma}_f(\mathbf{F}_e, \mathbf{D}) = \begin{cases}\mathbf{Q}^T\boldsymbol{\sigma}_f(\mathbf{Q}\mathbf{F}_e, \mathbf{Q}\mathbf{D}\mathbf{Q}^T)\mathbf{Q}; & \text{for each } \mathbf{Q}\in\Theta,\\ \boldsymbol{\sigma}_f(\mathbf{F}_e\mathbf{Q}, \mathbf{D}); & \text{for each } \mathbf{Q}\in\mathcal{G},\end{cases} \tag{4.29}$$

and

$$\boldsymbol{\sigma}_f\cdot\mathbf{D} \geqslant 0. \tag{4.30}$$

In similar fashion, the response equations for the fully isotropic model take the final form

$$\psi = \hat{\psi}(\mathbf{b}),$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}_f \begin{cases} \boldsymbol{\sigma}_e = 2\rho \dfrac{\partial \psi}{\partial \mathbf{b}} \mathbf{b}, \\ \boldsymbol{\sigma}_f = \hat{\boldsymbol{\sigma}}_f(\mathbf{b}, \mathbf{D}), \end{cases} \tag{4.31}$$

subject to frame invariance,

$$\begin{aligned} \hat{\psi}(\mathbf{b}) &= \hat{\psi}(\mathbf{Q}\mathbf{b}\mathbf{Q}^T) \\ \boldsymbol{\sigma}_f(\mathbf{b}, \mathbf{D}) &= \mathbf{Q}^T \boldsymbol{\sigma}_f(\mathbf{Q}\mathbf{b}\mathbf{Q}^T, \mathbf{Q}\mathbf{D}\mathbf{Q}^T)\mathbf{Q}; \qquad \text{for each } \mathbf{Q} \in \Theta, \end{aligned} \tag{4.32}$$

and the dissipation constraint (4.30).

B. *Dislocation strain*

Over the years, a number of theories have been introduced in an attempt to model material behavior over a range which extends beyond the elastic limit. These theories variously incorporate yield criteria, isotropic and/or anisotropic (kinematic) hardening rules and rate dependence through viscoplasticity and/or anelasticity. Almost all of these theories are intended to model polycrystalline metals or alloys which are probably best regarded as structurally isotropic. As a final exercise a general theory encompassing all of these theories shall be outlined. This general theory, called the theory of *dislocation strain*, is based on a crude model for the "strength" and "directionality" of the local dislocation distribution.

The first step in constructing a general theory is to parameterize the state space by selecting state variables. This must be viewed as a critical step which, in many respects, is analogous to the selection of colors for an artist's palette. This analogy is appropriate insofar as the choice of state variables circumscribes our ability to "detail" the intricacies of dislocation distribution and interaction. Moreover, if (for the sake of simplicity) only a few "colors" are to be selected, then their selection should be motivated by the desire to achieve the "best rendering" of the "subject".

For this structurally isotropic theory, reference cell placement is adequately characterized by the deformation tensor $\mathbf{c} = \mathbf{b}^{-1}$. The choice of $\mathbf{c}$ (as opposed to any other symmetric strain measure $\mathbf{e} = \hat{\mathbf{e}}(\mathbf{b})$) is based on the metric expression (3.46) which makes it possible to regard $\mathbf{c}$ as defining the elastic stretch ellipsoid in the current configuration. This interpretation follows from the fact that any solution $\boldsymbol{\lambda} = \lambda \hat{\boldsymbol{\lambda}}$ to the quadradic form

$$\boldsymbol{\lambda} \cdot \mathbf{c} \cdot \boldsymbol{\lambda} = 1 \tag{4.33}$$

gives the elastic stretch λ of the material element currently oriented in the $\hat{\boldsymbol{\lambda}}$ direction. With reference to $(3.40)_3$ and $(3.51)_2$, $\mathbf{c}$ is seen to evolve according to the rate form

$$\mathring{\mathbf{c}} = \mathbf{c}(\mathbf{d} - \mathbf{D}) + (\mathbf{d} - \mathbf{D})\mathbf{c}, \tag{4.34}$$

expressed in terms of a symmetric inelastic rate function $\mathbf{d}$ which must be specified in accordance with frame invariance through (3.36). Plastic deformation shall also be constrained to be isochoric so that

$$\rho = \rho_0 \sqrt{\det(\mathbf{c})}. \tag{4.35}$$

In view of (3.49) and (3.52) it is also evident that this gives rise to the differential rate constraint

$$\operatorname{tr}(\boldsymbol{\Lambda}_s) = \mathbf{b} \cdot \boldsymbol{\Gamma}_c = \operatorname{tr}(\mathbf{d}) = 0. \tag{4.36}$$

In this model dislocation distribution is described in terms of its "strength" and its "directionality". The isotropic characteristics of dislocation distribution which effect mechanical properties are described in terms of a single scalar *dislocation density* (per unit mass) parameter μ. This variable is generally associated with the size of yield surface through an isotropic hardening rule. In the classic isotropic hardening model of Hill[6], μ is assumed to be directly related to the accumulated plastic work (dissipated elastic strain energy). It is further assumed that the directionality (anisotropy) of the dislocation distribution can be adequately described, or pictured, in terms of a local dislocation ellipsoid defined in terms of a symmetric positive definite *dislocation strain tensor* $\mathbf{c}^*$ through an expression identical in form to (4.33). This ellipsoid is assumed to be materially embedded (as are the dislocations themselves) during a purely elastic deformation so that the $\mathbf{c}^*$ evolution equation can be expressed in the form

$$\mathring{\mathbf{c}}^* = \mathbf{c}^*(\mathbf{d}^* - \mathbf{D}) + (\mathbf{d}^* - \mathbf{D})\mathbf{c}^*, \tag{4.37}$$

in terms of a symmetric, inelastic dislocation rate function $\mathbf{d}^*$, subject to (3.36).

Various physical scenarios can be employed to motivate this approach to dislocation modeling, although none should be regarded in a strictly literal sense. One such device is to regard all possible dislocation distributions as being geometrically strained from one (of strength μ) which is spatially isotropic, with the metric relationship

$$\mathbf{X}_1^* \cdot \mathbf{X}_2^* = \mathbf{x}_1 \cdot \mathbf{c}^* \cdot \mathbf{x}_2 \tag{4.38}$$

defining the geometry of this "preferred" element configuration relative to the current. In order to remove the indeterminacy in the relative size of this configuration it seems reasonable to stipulate that it have the same mass density as the reference cell so that

$$\rho = \rho_0 \sqrt{\det(\mathbf{c}^*)} \to \operatorname{tr}(\mathbf{d}^*) = 0. \tag{4.39}$$

An alternative interpretation for this second strain measure is implicit in the Hart[1] model. This interpretation is based on the observation that sudden removal of supporting stress is generally accompanied by instantaneous (rate independent) elastic strain recovery followed by a period of additional elastic energy release and rate dependent strain recovery. The phenomenon of continued recovery, following the geometric "relaxation" of the reference cell, reflects the presence of what Hart calls "anelastic" or rate-dependent elastic strain which is a manifestation of a nonisotropic, nonequilibrium dislocation distribution. The rate dependent portion of the relaxation process results from the migration of dislocations, driven by internal back-stresses, towards an isotropic equilibrium distribution. Hart proposes that a tensor measure for this stored strain, which could presumably be determined from the instantaneous geometry of the local dislocation distribution, is fundamental to the determination of state. If it were not for the fact that the plastic deformation mechanism generally remains active, this anelastic strain could be identified with the total geometry change realized during the rate dependent portion of the relaxation process. As it is, the total elastic strain, defined as the sum of the current values of the elastic and anelastic strain, is used to define the instantaneous "plastically deformed" or preferred configuration relative to the current. The geometric difference between the instantaneous preferred configuration and the final rest configuration obtained after sudden stress removal corresponds to the additional plastic strain which accumulates during the relaxation process. Either of these descriptions is useful insofar as it motivates the fundamental assumption underpinning this theory, i.e. that the dislocation induced anisotropic characteristics of each unstressed element are similar to (no more complicated than) those of an isotropic elastic element subjected to an isochoric prestrain.

Having thus characterized the state space for this theory it remains only to place restrictions on the class of allowable stimuli and to specify functional smoothness properties. For the class of materials which exhibit initial elastic response it seems appropriate to allow any continuous, piecewise smooth stimuli with perhaps the added possibility of purely

elastic jumps, for which the state jump conditions

$$\begin{aligned} \mathbf{c}(t^+) &= (\mathbf{F}^{-1})^T \mathbf{c}(t^-)(\mathbf{F}^{-1}), \\ \mathbf{c}^*(t^+) &= (\mathbf{F}^{-1})^T \mathbf{c}^*(t^-)(\mathbf{F}^{-1}), \\ \mu(t^+) &= \mu(t^-) \end{aligned} \tag{4.40}$$

apply. It is further assumed that continuous stimuli elicit continuous response and that smooth stimuli give rise to smooth trajectories in state space. With reference to the general response and evolution forms (3.35), this general theory is seen to take the form

$$\begin{aligned} \psi &= \hat{\psi}(\mathbf{c}, \mathbf{c}^*, \mu), \\ \boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{c}, \mathbf{c}^*, \mu), \\ \dot{\mathbf{c}} &= \mathbf{c}(\mathbf{d}-\mathbf{D})+(\mathbf{d}-\mathbf{D})\mathbf{c}; \qquad \mathbf{d} = \hat{\mathbf{d}}(\mathbf{c}, \mathbf{c}^*, \mu, \mathbf{D}) = \mathbf{d}^T, \\ \dot{\mathbf{c}}^* &= \mathbf{c}^*(\mathbf{d}^*-\mathbf{D})+(\mathbf{d}^*-\mathbf{D})\mathbf{c}^*; \qquad \mathbf{d}^* = \hat{\mathbf{d}}^*(\mathbf{c}, \mathbf{c}^*, \mu, \mathbf{D}) = (\mathbf{d}^*)^T, \\ \dot{\mu} &= \nu(\mathbf{c}, \mathbf{c}^*, \mu, \mathbf{D}), \end{aligned} \tag{4.41}$$

in terms of the response functions $\hat{\psi}$ and $\hat{\boldsymbol{\sigma}}$, and the inelastic evolution functions $\hat{\mathbf{d}}$, $\hat{\mathbf{d}}^*$ and ν. In view of the frame invariance requirement (3.36) it is clear that all response and evolution functions ($\hat{\psi}$, $\hat{\boldsymbol{\sigma}}$, $\hat{\mathbf{d}}$, $\hat{\mathbf{d}}^*$ and ν) must be isotropic functions of their full set of tensor arguments. In addition, the evolution of the deformation tensors $\mathbf{c}$ and $\mathbf{c}^*$ is constrained by the geometric requirement that

$$\rho/\rho_0 = \sqrt{\det(\mathbf{c})} = \sqrt{\det(\mathbf{c}^*)} \to \operatorname{tr}(\mathbf{d}) = \operatorname{tr}(\mathbf{d}^*) = 0. \tag{4.42}$$

Yield criteria can be added by specifying an additional isotropic scalar yield function f which determines an elastic region

$$E = \{(\mathbf{c}, \mathbf{c}^*, \mu) : f(\mathbf{c}, \mathbf{c}^*, \mu) < 0\} \tag{4.43}$$

in state space. This elastic region is necessarily characterized by vanishing inelastic rates, i.e.

$$[\hat{\mathbf{d}}, \hat{\mathbf{d}}^*, \nu] = 0 \qquad \text{whenever } (\mathbf{c}, \mathbf{c}^*, \mu) \in E, \tag{4.44}$$

and a yield surface

$$\partial E = \{(\mathbf{c}, \mathbf{c}^*, \mu) : f(\mathbf{c}, \mathbf{c}^*, \mu) = 0\} \tag{4.45}$$

on which additional elastic, neutral, and plastic loading criteria must be specified.

Some other physical features that are incorporated into existing models are the invariance of elastic properties, rate independence and a fast rate elastic limit. The invariance of elastic properties is explicit in the standard isotropic and kinematic hardening plasticity models insofar as stress is assumed to be related to the instantaneous elastic strain through Hooke's law, with the dislocation state variables effecting only the inelastic mechanisms. In the context of this general theory this assumption allows for the simplified response forms

$$\begin{aligned} \psi &= \hat{\psi}(\mathbf{c}), \\ \boldsymbol{\sigma} &= \hat{\boldsymbol{\sigma}}(\mathbf{c}). \end{aligned} \tag{4.46}$$

Full rate independence is also explicit in many existing models. This is guaranteed by

requiring that the inelastic rate functions be homogeneous, degree one in **D** in the sense that

$$h(\mathbf{c}, \mathbf{c}^*, \mu, \kappa\mathbf{D}) = \kappa[h(\mathbf{c}, \mathbf{c}^*, \mu, \mathbf{D})]. \tag{4.47}$$

The rate dependent theory of Hart represents an attempt to replace explicit yield criteria with certain types of limit behavior. One such device seems to be a fast rate elastic limit which assures that a given deformation becomes purely elastic in the limit as the deformation time approaches zero. This limit has recently been considered in [7] (in connection with a similar state variable model for elastic fluids) wherein it is established that the desired limit behavior results from the requirement that all inelastic rate functions $(\hat{\mathbf{d}}, \hat{\mathbf{d}}^*, \nu)$ satisfy

$$\lim_{D\to\infty} (1/D)[h(\mathbf{c}, \mathbf{c}^*, \mu, \mathbf{D})] = 0; \qquad D \equiv \|\mathbf{D}\|. \tag{4.48}$$

A particularly simple way to achieve this is by eliminating the dependence on **D**. This is a characteristic of the Hart model as well as the aforementioned elastic fluid model.

Apart from these subsidiary restrictions, specification of the response and evolution functions is necessarily subject to the second law of thermodynamics through the dissipation inequality which, for this theory, takes the form:

$$\begin{gathered}
\boldsymbol{\sigma}\cdot\mathbf{D} - \rho\dot{\psi} \geqslant 0, \\
\boldsymbol{\sigma}\cdot\mathbf{D} - \rho\left\{\frac{\partial\psi}{\partial\mathbf{c}}\cdot[\mathbf{c}(\mathbf{d}-\mathbf{D})+(\mathbf{d}-\mathbf{D})\mathbf{c}] + \frac{\partial\psi}{\partial\mathbf{c}^*}\cdot[\mathbf{c}(\mathbf{d}^*-\mathbf{D})+(\mathbf{d}^*-\mathbf{D})\mathbf{c}^*] + \frac{\partial\psi}{\partial\mu}\nu\right\} \geqslant 0, \\
\left\{\boldsymbol{\sigma} + 2\rho\ \mathrm{sym}\left[\frac{\partial\psi}{\partial\mathbf{c}}\mathbf{c} + \frac{\partial\psi}{\partial\mathbf{c}^*}\mathbf{c}^*\right]\right\}\cdot\mathbf{D} - 2\rho\ \mathrm{sym}\left(\frac{\partial\psi}{\partial\mathbf{c}}\mathbf{c}\right)\cdot\mathbf{d} - 2\rho\ \mathrm{sym}\left(\frac{\partial\psi}{\partial\mathbf{c}^*}\mathbf{c}^*\right)\cdot\mathbf{d}^* - \rho\frac{\partial\psi}{\partial\mu}\nu \geqslant 0.
\end{gathered} \tag{4.49}$$

Since **D** may be specified independently as one proceeds from a given state, the conclusion that

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}^* \begin{cases} \boldsymbol{\sigma}_e = -2\rho\ \mathrm{sym}\left(\dfrac{\partial\psi}{\partial\mathbf{c}}\mathbf{c}\right), \\ \boldsymbol{\sigma}^* = -2\rho\ \mathrm{sym}\left(\dfrac{\partial\psi}{\partial\mathbf{c}^*}\mathbf{c}^*\right), \end{cases} \tag{4.50}$$

$$\boldsymbol{\sigma}_e\cdot\mathbf{d} + \boldsymbol{\sigma}^*\cdot\mathbf{d}^* - \rho\frac{\partial\psi}{\partial\mu}\nu \geqslant 0$$

follows either from the imposition of the fast rate elastic limit or a classical yield criteria wherein each accessible state is a limit point of the open elastic region E.

At this point a number of familiar special cases (albeit in a generalized large strain form) are apparent. First of all, isotropic hyperelasticity clearly follows from the invariance of elastic properties and the choice $\hat{\mathbf{d}} = 0$. The rate independent, isotropic hardening plasticity model of Hill follows from the invariance of elastic properties, an elastic region E defined by

$$E = \{(\mathbf{c}, \mu) : f(\mathbf{s}) < \kappa(\mu)\}, \tag{4.51}$$

in terms of an isotropic yield function f of an isotropic elastic stress function $\mathbf{s} = \hat{\mathbf{s}}(\mathbf{c})$, and a monotonic hardening function κ of μ. The selection of a symmetric, deviatoric, isotropic inelastic deformation rate function

$$\mathbf{d} = \hat{\mathbf{d}}(\mathbf{c}, \mu, \mathbf{D}) \tag{4.52}$$

must be consistent with rate independence, the dissipation inequality $(4.50)_2$, and vanish identically in the elastic region. In [8] it is established that the requirement of stability in the sense of Il'iushin determines the choice

$$\mathbf{s} = \operatorname{dev}(\boldsymbol{\tau}) = \boldsymbol{\tau} - \tfrac{1}{3}\mathbf{I}\ \operatorname{tr}(\boldsymbol{\tau}), \tag{4.53}$$

in terms of the Kirchhoff stress $\boldsymbol{\tau} = (\rho_0/\rho)\boldsymbol{\sigma}$, as well as convexity of the yield surface in stress space and the familiar normality condition

$$\mathbf{d} = \alpha[\partial f / \partial \boldsymbol{\tau}]. \tag{4.54}$$

The familiar kinematic hardening theory is also characterized by the invariance of elastic properties and rate independence. The elastic region E is defined by

$$E = \{(\mathbf{c}, \mathbf{c}^*) : f(\mathbf{s} - \boldsymbol{\alpha}) < 0\} \tag{4.55}$$

in terms of an isotropic yield function f, an isotropic elastic stress function $\mathbf{s} = \hat{\mathbf{s}}(\mathbf{c})$, and a symmetric, isotropic, inelastic "back-stress" function $\boldsymbol{\alpha} = \hat{\boldsymbol{\alpha}}(\mathbf{c}, \mathbf{c}^*)$. The symmetric, deviatoric, isotropic inelastic deformation rate functions

$$\begin{aligned} \mathbf{d} &= \hat{\mathbf{d}}(\mathbf{c}, \mathbf{c}^*, \mathbf{D}), \\ \mathbf{d}^* &= \hat{\mathbf{d}}^*(\mathbf{c}, \mathbf{c}^*, \mathbf{D}) \end{aligned} \tag{4.56}$$

must again be homogeneous, degree one in $\mathbf{D}$, vanish identically in the elastic region, and satisfy the dissipation inequality $(4.50)_2$. Variants of this model shall be considered in a subsequent publication.

Although not immediately apparent, the constitutive forms presently employed by Hart can be shown to derive from a "small strain" linearization of the forms

$$\begin{aligned} &\psi = \hat{\psi}(\mathbf{c}, \mathbf{c}^*), \\ &\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}^* \begin{cases} \boldsymbol{\sigma}_e = -2\rho\ \operatorname{sym}\left(\dfrac{\partial \psi}{\partial \mathbf{c}}\mathbf{c}\right), \\ \boldsymbol{\sigma}^* = -2\rho\ \operatorname{sym}\left(\dfrac{\partial \psi}{\partial \mathbf{c}^*}\mathbf{c}^*\right), \end{cases} \\ &\mathbf{d} = \hat{\mathbf{d}}(\mathbf{c}, \mathbf{c}^*, \mu) = \alpha\ \operatorname{dev}(\boldsymbol{\sigma}_e); \qquad \alpha = \hat{\alpha}(\mathbf{c}, \mathbf{c}^*, \mu), \\ &\mathbf{d} = \hat{\mathbf{d}}^*(\mathbf{c}, \mathbf{c}^*, \mu) = \beta\ \operatorname{dev}(\boldsymbol{\sigma}^*); \qquad \beta = \hat{\beta}(\mathbf{c}, \mathbf{c}^*, \mu), \end{aligned} \tag{4.57}$$

subject to the additional stress/energy constraint that $\boldsymbol{\sigma} = 0$ if and only if $\mathbf{c} = \mathbf{I}$.

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