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PLASTICITY THEORY FORMULATED IN TERMS OF PHYSICALLY BASED MICROSTRUCTURAL VARIABLES—PART I. THEORY

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Abstract—In the present paper a theory for elastic–plastic materials is developed that is valid for general anisotropic response and is independent of the choice of the reference configuration from which total strain is measured. Also, the constitutive equation for stress is hyperelastic. The main idea is to focus attention on the current physical state of the material as characterized by the current state of the microstructure in general and the atomic lattice in particular. Here it is assumed that the elastic response of the atomic lattice remains unaffected by previous material processing. This means that the lattice state of the material when it is macroscopically stress-free and at some reference temperature can be used as a reference state for determining elastic deformations of the lattice. To this end, a vector triad \mathbf{m} , is introduced which models the orientation and elastic deformation of the average atomic lattice in the present state, relative to this constant reference lattice state. Anisotropies of the material response are referred to the vectors \mathbf{m}_i , which in principle, are measurable in the present physical state. Even for elastic materials, this approach seems to clarify the explicit dependence of anisotropy on identifiable material directions in the present state. Furthermore, effects of texturing causing alignment of the triad due to material processing can be modeled.

1. INTRODUCTION

This paper is mainly concerned with the physics of plastic flow of crystalline metals. In particular, it is recalled that a macroscopic piece of a crystalline metal is composed of millions of atoms which are arranged in reasonably structured atomic lattices. In general, the atomic lattices contain a number of defects which may aid or inhibit plastic flow of the metal. From the macroscopic continuum point of view, a material point represents a small region of space which contains a very large number of atoms. Furthermore, two neighboring material points constitute a macroscopic material line element like $d\mathbf{X}$ associated with the fixed reference configuration or $d\mathbf{x}$ associated with the present configuration.

During large deformation plastic flow dislocations move through the atomic lattice causing atoms to migrate through the lattice so that the nearest neighbors of an individual atom change with time. This means that during plastic flow atoms may move from one macroscopic material point to another. Of course, if the flow of atoms in and out of a macroscopic continuum material point is balanced, then aspects of this physical feature may be ignored in the continuum mechanics formulation. However, it is important to emphasize that because of this flow of atoms neither of the macroscopic material line elements $d\mathbf{X}$ or $d\mathbf{x}$ can be easily related to the current state of the atomic lattice.

In spite of the large total deformations that can occur during plastic flow, the atomic lattice remains reasonably undistorted. In fact, it is usually assumed that the dilatation and distortion of the atomic lattice are elastic and that they are the direct cause of stresses that occur in the metal.

Recent reviews of theories for continuum plasticity (Naghdi, 1990) and crystal plasticity (Asaro, 1983) indicate that constitutive equations for large deformation of elastic–plastic materials are still in a state of development. Constitutive equations for elastic–plastic materials can be developed by introducing a symmetric plastic deformation tensor \mathbf{C}_p or plastic strain tensor [e.g. Green and Naghdi (1965)], by introducing a nonsymmetric plastic deformation tensor \mathbf{F}_p [e.g. see Green and Naghdi (1965, footnote, p. 260); Lee and Liu (1967); Lee (1969); Rice (1971); Mandel (1973); Dafalias (1985); Loret (1983)], or by

introducing a nonsymmetric elastic deformation tensor \mathbf{F}_e [e.g. Besseling (1968)], each of which is determined by an evolution equation for its time rate of change. In these developments: \mathbf{C}_p is referred to the reference configuration; \mathbf{F}_p is referred to both the reference configuration and an intermediate configuration; \mathbf{F}_e is referred to both an intermediate and the present configuration. Due to the controversial nature of issues related to the proper invariance under superposed rigid body motions and generality of these theories, it is preferable to first develop the present theory and only later in a discussion section relate it to relevant existing theories.

In this work attention is focused on the following two physical problems with common constitutive theories for elastic–plastic media.

- (P1) Anisotropic hyperelastic formulations of constitutive equations for both elastic and elastic–plastic materials require the functional form of the Helmholtz free energy ψ to be explicitly dependent on the particular choice of the reference or intermediate configurations.
- (P2) Plastic deformation from the reference configuration cannot be measured given the present state of the material alone (Gilman, 1960, p. 99).

The main physical implication of the first problem (P1) is that in order to use a specific functional form for ψ it is necessary to somehow determine relevant information about the particular choice of the reference or intermediate configuration which was used to determine the material parameters that characterize the functional form. Even for an elastic material which is stress-free and at temperature θ_0 in the reference configuration it is impossible to determine the absolute orientation of the reference configuration from knowledge of the present state of the material alone. This emphasizes the need for the constitutive description of an anisotropic material to be explicitly dependent on material directions which can be identified in the present state of the material. For elastic–plastic materials this problem is even more severe because the stress-free shape of a homogeneously deformed material changes as plastic deformation occurs.

The second problem (P2) is directly related to the problem of determining the reference or intermediate configurations. However, (P2) manifests itself in a practical way because it is necessary to specify initial conditions for \mathbf{C}_p , \mathbf{F}_p or \mathbf{F}_e in order to integrate the evolution equations for their time rates of change.

The main objective of this paper is to develop a theory for elastic–plastic materials that is valid for general anisotropic response and is independent of the choice of the reference configuration from which total strain is measured. In particular, a theory will be proposed which avoids the two physical problems (P1) and (P2) discussed above. Moreover, the proposed theoretical structure explicitly connects anisotropic material response with identifiable directions in the present material state. Although, the present work is motivated by the physical discussions of Besseling (1968) and Mandel (1973), the resulting theoretical formulation is different from that proposed by either of these authors. A detailed comparison with relevant existing theories will be presented in the discussion section after the present theory has been developed.

Specifically, the present theory uses the idea proposed by Eckart (1948), and modified by Besseling (1968), that an evolution equation for elastic deformation can be specified which includes the relaxation effects of plastic deformation without introducing a plastic deformation tensor explicitly. Also, the present theory uses the idea of Mandel (1973) that elastic anisotropies can be described with reference to a triad of vectors. In addition, the theory uses the idea argued by both Besseling (1968) and Mandel (1973) that the rotation and deformation of the atomic lattice is not directly related to the total deformation (relative to the reference configuration) of a continuum material element.

The theory is developed by focusing attention on the current physical state of the material as characterized by the current state of the microstructure in general, and the atomic lattice in particular. As the material deforms, the atomic lattice and microstructure rotate and deform. Here it is assumed that the elastic response of the atomic lattice remains unaffected by previous material processing even though dislocation and defect generation and annihilation may cause changes in the resistance to plastic flow. This means that the

lattice state of the material, when it is macroscopically stress-free and at some reference temperature θ_0 , can be used as a reference state for determining elastic deformations of the lattice. For convenience this Reference Lattice State is denoted by the abbreviation RLS.

To formulate the theory, a triad of vectors \mathbf{m}_i ($i = 1, 2, 3$) is introduced (at each material point) which characterizes the dilatation, distortion and orientation of the average atomic lattice in the present state relative to the RLS. These microstructural variables are determined by evolution equations of the form

$$\dot{\mathbf{m}}_i = \mathbf{L}_m \mathbf{m}_i, \quad (1)$$

where the second-order tensor \mathbf{L}_m requires a constitutive equation which includes plastic relaxation effects, and a superposed dot denotes material time differentiation holding the location \mathbf{X} of a material point in the reference configuration fixed. Since the vectors \mathbf{m}_i are directly related to the present state of the atomic lattice, the initial values of \mathbf{m}_i required to integrate (1) can, in principle, be measured in the present state. Furthermore, since the vectors \mathbf{m}_i characterize the atomic lattice, they are not directly connected to the material line elements $d\mathbf{X}$ or $d\mathbf{x}$, which is consistent with the fact that during plastic flow atoms migrate through the atomic lattice.

The explicit use of the vectors \mathbf{m}_i as a basis for tensors referred to the present configuration has two main advantages over direct formulations: (A1) material anisotropies characterized by functions of these components are explicitly specified in terms of directions that can be determined by the orientation of the material in its present state. These directions are independent of the particular choice of the reference or intermediate configurations because \mathbf{m}_i characterize material (lattice) directions which, in principle, are measurable in the present state; (A2) these components are trivially invariant under superposed rigid body motions (hereafter denoted by SRBM) so that arbitrary functions of these components may be specified without effecting proper invariance under SRBM.

It will be shown that the present development produces an approach to the formulation of constitutive equations for nonlinear elastic response which retains the advantage (A1). Specifically, the resulting equations for nonlinear elastic response are not formulated in terms of the deformation gradient from the reference configuration and they do not depend on the particular choice of the reference configuration.

In the following sections the microstructural variables that are used to characterize the elastic deformation (relative to the RLS) and orientation of the atomic lattice in its present state are described. After briefly reviewing the thermodynamical framework within which restrictions on the constitutive equations are developed, general constitutive equations for both rate-dependent elastic-viscoplastic response and rate-independent elastic-plastic response are discussed. Then, the special cases of elastically isotropic response and small elastic deformations are discussed, and the relationship of the present theory to other existing theories in the literature is presented. In a companion paper (Rubin, 1994) specific constitutive equations and examples of the response to large deformation uniaxial stress, simple shear and isochoric extension are presented.

Throughout the text: tensors are denoted by bold faced symbols; the dot product $\mathbf{A} \cdot \mathbf{B}$ between two tensors denotes the usual scalar product when \mathbf{A} , \mathbf{B} are vectors and it denotes the scalar $\text{tr}(\mathbf{A}\mathbf{B}^T)$ when \mathbf{A} and \mathbf{B} are second-order tensors; the notation $\mathbf{A} \times \mathbf{B}$ denotes the usual cross product between two vectors \mathbf{A} , \mathbf{B} ; the symbol \otimes denotes the tensor product between two tensors; the usual summation convention for repeated indices is implied except for the indices (e, p, m) which are used to denote specific tensors.

2. THE MICROSTRUCTURAL VARIABLES

Here, a simple continuum model is considered which focuses attention on the current orientation and elastic deformation of the average atomic lattice. As mentioned in the introduction, the stress-free state of the atomic lattice at reference temperature θ_0 can be used as a Reference Lattice State (RLS) for characterizing deformation of the atomic lattice. In this regard, it is well known (Richman, 1967, p. 30) that the unit cells of the

Bravais lattices can be characterized by three atomic lengths and three atomic angles which determine a parallelepiped. Alternatively, the state of an atomic lattice (or the parallelepiped) in the RLS can be characterized by a right-handed triad of three linearly independent vectors \mathbf{D}_i (with $\mathbf{D}_1 \times \mathbf{D}_2 \cdot \mathbf{D}_3 > 0$) which have the dimensions of length and are measured relative to a fixed right-handed set of orthonormal base vectors \mathbf{e}_i . Since \mathbf{D}_i are not orthonormal vectors it is convenient to define the reciprocal vectors \mathbf{D}^i by

$$\mathbf{D}^i \cdot \mathbf{D}_j = \delta_j^i, \quad (2)$$

where δ_j^i is the Kronecker delta symbol. Furthermore, let \mathbf{d}_i be the right-handed triad of three linearly independent vectors characterizing the parallelepiped associated with the present state of the atomic lattice.

Next, the three vectors \mathbf{m}_i are introduced which are microstructural variables that represent the current state of the atomic lattice and are defined by

$$\mathbf{m}_i = (\mathbf{d}_i \otimes \mathbf{D}^i) \mathbf{e}_i. \quad (3)$$

It follows that \mathbf{m}_i are a right-handed set of linearly independent unitless vectors having the property that

$$m^{1/2} = \mathbf{m}_1 \times \mathbf{m}_2 \cdot \mathbf{m}_3 = \frac{\mathbf{d}_1 \times \mathbf{d}_2 \cdot \mathbf{d}_3}{\mathbf{D}_1 \times \mathbf{D}_2 \cdot \mathbf{D}_3} > 0, \quad (4)$$

which shows that $m^{1/2}$ is the ratio of the volumes of the parallelepipeds defining the present state and RLS of the atomic lattice. Since \mathbf{m}_i are not necessarily orthonormal vectors it is convenient to introduce the reciprocal vectors \mathbf{m}^i and the positive definite metrics m_{ij} , m^{ij} , such that

$$\mathbf{m}^i \cdot \mathbf{m}_j = \delta_j^i, \quad m_{ij} = \mathbf{m}_i \cdot \mathbf{m}_j, \quad m^{ij} = \mathbf{m}^i \cdot \mathbf{m}^j. \quad (5a, b, c)$$

Furthermore, since m_{ij} is a positive definite matrix, its unique square root n_{ij} and the inverse n^{ij} of its square root exist satisfying the equations

$$m_{ij} = n_{ir} n_{rj}, \quad n_{ij} = n_{ji}, \quad n^{ir} n_{rj} = \delta_j^i. \quad (6a, b, c)$$

It then follows from (5) and (6) that, since n_{ij} is uniquely determined by m_{ij} , an orthonormal set of vectors \mathbf{a}_i may be defined uniquely in terms of \mathbf{m}_i by the formulas

$$\mathbf{m}_i = n_{ir} \mathbf{a}_r, \quad \mathbf{a}_i = n^{ir} \mathbf{m}_r, \quad \mathbf{a}_i \cdot \mathbf{a}_j = \delta_{ij}. \quad (7a, b, c)$$

Since it has been assumed that the relative dimensions of the atomic lattice in an RLS are independent of material processes, it follows that in any RLS the vectors \mathbf{d}_i are related to the associated vectors \mathbf{D}_i by a proper orthogonal tensor \mathbf{R} such that

$$\mathbf{d}_i = \mathbf{R} \mathbf{D}_i, \quad \mathbf{R} \mathbf{R}^T = \mathbf{I}, \quad \det \mathbf{R} = 1, \quad (8a, b, c)$$

where \mathbf{I} is the unit tensor. Consequently, with the help of (3), (5) and (8) it follows that

$$m_{ij} = \delta_{ij} \quad \text{in any RLS.} \quad (9)$$

Within the context of the above characterization of the atomic lattice, the vectors \mathbf{d}_i can, in principle, be measured in the present state (at nonzero stress and general temperature θ) using X-ray diffraction techniques. This means that the relevant features of the RLS can also be measured. Thus, the present values of \mathbf{m}_i can, in principle, be measured. Then, using

(7) the present values of \mathbf{a}_i can also be measured and used to characterize the present orientation of the atomic lattice.

Above, the use of a triad of vectors \mathbf{m}_i was motivated to describe the dilatation and distortion of a single atomic lattice. This notion can be generalized by assuming that the vectors \mathbf{m}_i are simple continuum representations of the average atomic lattice at a material point. From a microscopic point of view, the atomic lattice may be inhomogeneous because individual unit cells can be locally distorted by the presence of dislocations and other defects. This means that the values of \mathbf{m}_i associated with a macroscopic material point represent average properties of a region that includes a large number of atoms. Similarly, with reference to polycrystalline materials or granular materials, the values of \mathbf{m}_i represent average properties of a region that includes a large number of crystals or grains. At present, the specific averaging process used to define \mathbf{m}_i in terms of the current physical lattice state is left undefined even though it is assumed that both the magnitudes and directions of \mathbf{m}_i associated with the present state of the material can be uniquely determined. Consequently, it is assumed that the present values of \mathbf{m}_i can, in principle, be measured. In this regard, it should be mentioned that the identification of \mathbf{m}_i depends on the specific constitutive equations that are used to predict material response. Thus, within the context of specific constitutive assumptions one must search for features of the material response which help characterize \mathbf{m}_i . For example, one can use the directions \mathbf{a}_i (defined uniquely by \mathbf{m}_i) to characterize anisotropies of the material in its present state. This characterization is physically appealing because the anisotropies are referred to directions which are determined by the present state of the material instead of relative to directions associated with the specification of an arbitrary reference configuration.

With reference to SRBM the value of a quantity in the superposed configuration is denoted by the same symbol with a superposed (+). Since \mathbf{m}_i are measured in the present state, which is associated with the present configuration, it follows that under SRBM

$$\mathbf{m}_i^+ = \mathbf{Q}\mathbf{m}_i, \quad (10)$$

where $\mathbf{Q}(t)$ is an arbitrary proper orthogonal tensor function of time t . Thus, with the help of (3), (5), (7), (10) and the knowledge that \mathbf{D}_i and \mathbf{e}_i are unaffected by SRBM it can be shown that under SRBM the quantities m_{ij} , \mathbf{d}_i and \mathbf{a}_i transform by

$$m_{ij}^+ = m_{ij}, \quad \mathbf{d}_i^+ = \mathbf{Q}\mathbf{d}_i, \quad \mathbf{a}_i^+ = \mathbf{Q}\mathbf{a}_i. \quad (11a, b, c)$$

Also, using eqn (10) and the evolution equation (1) it follows that under SRBM, \mathbf{L}_m must transform by

$$\mathbf{L}_m^+ = \mathbf{Q}\mathbf{L}_m\mathbf{Q}^T + \mathbf{\Omega}, \quad (12)$$

where $\mathbf{\Omega}$ is the skew-symmetric tensor defined by

$$\mathbf{\Omega} = \dot{\mathbf{Q}}\mathbf{Q}^T = -\mathbf{\Omega}^T. \quad (13)$$

3. THERMODYNAMICAL FORMULATION

By way of background, let \mathbf{X} be the location of a material point in an arbitrary but fixed reference configuration; \mathbf{x} be the location of the same material point in the current configuration at time t ; $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$ be the total deformation gradient; $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ be the right Green total deformation tensor; θ be the positive absolute temperature with reference value θ_0 . This section briefly reviews the main features of the thermodynamical procedures proposed by Green and Naghdi (1977, 1978, 1984) for general deformable media. Within the context of this formulation the usual laws of conservation of mass, and balances of

linear and angular momentum, and energy are supplemented by a balance law of entropy which in local form becomes

$$\rho\dot{\eta} = \rho(s + \xi) - \text{div } \mathbf{p}, \quad (14)$$

where ρ is the mass density per unit present volume, η is the specific entropy, s is the specific external rate of supply of entropy, ξ is the specific rate of internal production of entropy and \mathbf{p} is the entropy flux vector per unit present area. Furthermore, the quantities s and \mathbf{p} are related to the specific external rate of heat supply r , and the heat flux vector \mathbf{q} per unit present area by the formulas

$$s = \frac{r}{\theta}, \quad \mathbf{p} = \frac{\mathbf{q}}{\theta}. \quad (15a, b)$$

In general, ξ may be separated into two parts

$$\rho\theta\xi = -\mathbf{p} \cdot \mathbf{g} + \rho\theta\xi', \quad (16)$$

where $\mathbf{g} = \partial\theta/\partial\mathbf{x}$ is the temperature gradient with respect to the present position.

Letting ε denote the specific internal energy, the local equation for entropy (14) can be used to rewrite the local equation for energy in terms of the specific Helmholtz free energy $\psi = \varepsilon - \theta\eta$, such that

$$\rho(\dot{\psi} + \eta\dot{\theta}) - \mathbf{T} \cdot \mathbf{D} + \rho\theta\xi' = 0, \quad (17)$$

where \mathbf{T} is the Cauchy stress and \mathbf{D} is the symmetric part of the velocity gradient \mathbf{L} defined by

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \mathbf{D} + \mathbf{W}, \quad (18a)$$

$$\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T) = \mathbf{D}^T, \quad \mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T) = -\mathbf{W}^T. \quad (18b, c)$$

Also, in (17) the reduced form of balance of angular momentum has been used which requires \mathbf{T} to be symmetric

$$\mathbf{T}^T = \mathbf{T}. \quad (19)$$

In general, constitutive equations must be specified for the quantities

$$\{\psi, \eta, \xi', \mathbf{T}, \mathbf{p}\}, \quad (20)$$

and constitutive restrictions are obtained by demanding that the reduced forms of the energy equation (17) and the balance of angular momentum (19) be satisfied for all thermomechanical processes. Additional restrictions due to the second law of thermodynamics (Rubin, 1992) require

$$-\mathbf{q} \cdot \mathbf{g} > 0 \quad \text{for } \mathbf{g} \neq 0, \quad \frac{\partial\varepsilon}{\partial\theta} > 0, \quad \rho\theta\xi' \geq 0 \quad (21a, b, c)$$

to be satisfied for all thermomechanical processes. The restriction: (21a) requires heat to flow from hot to cold; (21b) requires the specific heat to be positive; (21c) requires nonideal material response to be dissipative.

4. CONSTITUTIVE EQUATIONS

From a constitutive point of view, it is assumed that the variables \mathbf{m}_i are determined by the evolution equation (1) for the rates $\dot{\mathbf{m}}_i$. In order to discuss a rather general set of constitutive equations for anisotropic elastic–plastic materials it is desirable to introduce additional hardening variables which characterize the resistance to plastic flow and which are also determined by evolution equations. For the present purposes, it suffices to examine the structure of the theory by introducing a scalar measure of isotropic hardening κ and a symmetric second-order tensorial measure of directional hardening $\boldsymbol{\beta}$, such as that introduced by Bodner (1985) to model the Bauschinger effect. Both κ and $\boldsymbol{\beta}$ are specified by constitutive equations for their rates $\dot{\kappa}$, $\dot{\boldsymbol{\beta}}$.

Before discussing general forms of the constitutive equations for the rates $\{\dot{\mathbf{m}}_i, \dot{\kappa}, \dot{\boldsymbol{\beta}}\}$ it is convenient to first consider certain restrictions on the constitutive equations due to invariance under SRBM. To this end, it is assumed that the quantities $\{\theta, \kappa, \boldsymbol{\beta}\}$ transform under SRBM by

$$\theta^+ = \theta, \quad \kappa^+ = \kappa, \quad \boldsymbol{\beta}^+ = \mathbf{Q}\boldsymbol{\beta}\mathbf{Q}^T. \tag{22a, b, c}$$

The invariance properties of \mathbf{m}_i have already been discussed [see eqn (10)]. Next, it is assumed that the Helmholtz free energy ψ is a function of the variables

$$\{\mathbf{m}_i, \theta, \kappa, \boldsymbol{\beta}\}. \tag{23}$$

Since \mathbf{m}_i are linearly independent, the tensor $\boldsymbol{\beta}$ may be represented in terms of its covariant components β_{ij} relative to the basis \mathbf{m}_i , such that

$$\boldsymbol{\beta} = \beta_{ij} \mathbf{m}^i \otimes \mathbf{m}^j, \quad \beta_{ij} = \boldsymbol{\beta} \cdot (\mathbf{m}_i \otimes \mathbf{m}_j). \tag{24a, b}$$

Thus, without loss in generality, the set of variables (23) may be replaced by the alternative set

$$\{\mathbf{m}_i, \theta, \kappa, \beta_{ij}\}. \tag{25}$$

Furthermore, using the properties (10), (22c) and (24b) it may easily be shown that

$$\beta_{ij}^+ = \beta_{ij}. \tag{26}$$

Then, invariance under SRBM requires the functional form of ψ to be restricted by

$$\psi = \hat{\psi}(\mathbf{m}_i, \theta, \kappa, \beta_{ij}) = \hat{\psi}(\mathbf{Q}\mathbf{m}_i, \theta, \kappa, \beta_{ij}) = \psi^+, \tag{27}$$

for arbitrary proper orthogonal \mathbf{Q} . The necessary and sufficient condition for ψ to satisfy this restriction is that ψ be an arbitrary function of the variables

$$\mathcal{V} = \{m_{ij}, \theta, \kappa, \beta_{ij}\}. \tag{28}$$

Recall now that the velocity gradient \mathbf{L} , its symmetric part \mathbf{D} , and its skew-symmetric part \mathbf{W} transform under SRBM by

$$\mathbf{L}^+ = \mathbf{Q}\mathbf{L}\mathbf{Q}^T + \boldsymbol{\Omega}, \quad \mathbf{D}^+ = \mathbf{Q}\mathbf{D}\mathbf{Q}^T, \quad \mathbf{W}^+ = \mathbf{Q}\mathbf{W}\mathbf{Q}^T + \boldsymbol{\Omega}, \tag{29a, b, c}$$

where $\boldsymbol{\Omega}(t)$ is defined by (13).

For an elastic–plastic material it is assumed that the constitutive equation for $\dot{\mathbf{m}}_i$ is given in the form (1) where \mathbf{L}_m is a second-order tensor function of the variables

$$\{\mathcal{V}, \mathbf{m}_i; \mathbf{L}, \dot{\theta}\}, \quad (30)$$

and the variables \mathbf{L} and $\dot{\theta}$ are included to allow for the possibility of describing rate-independent response. Thus, without loss in generality, \mathbf{L}_m may be separated additively into the form

$$\mathbf{L}_m = \mathbf{L} - \mathbf{L}_p, \quad (31)$$

where \mathbf{L}_p is a function of the same variables (30). However, in view of the transformation relations (12) and (29) it follows that \mathbf{L}_p transforms by

$$\mathbf{L}_p^+ = \mathbf{Q}\mathbf{L}_p\mathbf{Q}^T. \quad (32)$$

Furthermore, using the restriction (32) it can be shown that \mathbf{L}_p cannot depend on \mathbf{W} and that it must be a function of the form

$$\mathbf{L}_p = L_{p_{ij}}(\mathcal{V}; D_{ij}, \dot{\theta})\mathbf{m}^i \otimes \mathbf{m}^j, \quad (33)$$

where $L_{p_{ij}}$ and D_{ij} are the covariant components of \mathbf{L}_p and \mathbf{D} , respectively, relative to the basis \mathbf{m}_i ,

$$L_{p_{ij}} = \mathbf{L}_p \cdot (\mathbf{m}_i \otimes \mathbf{m}_j), \quad D_{ij} = \mathbf{D} \cdot (\mathbf{m}_i \otimes \mathbf{m}_j). \quad (34a, b)$$

Also, it may be shown that $L_{p_{ij}}$ and D_{ij} transform by

$$L_{p_{ij}}^+ = L_{p_{ij}}, \quad D_{ij}^+ = D_{ij}. \quad (35a, b)$$

The physical meaning of the separation (31) will be discussed after restrictions on the proposed constitutive assumptions have been developed.

In the following, constitutive equations for the rates $\{\dot{\mathbf{m}}_i, \dot{\kappa}, \dot{\beta}_{ij}\}$ are proposed which characterize both rate-dependent elastic-viscoplastic materials without a yield surface, and rate-independent elastic-plastic materials with a yield surface. For both types of materials it is assumed that $\dot{\mathbf{m}}_i$ is given by (1) with \mathbf{L}_m represented in the form (31), and that \mathbf{L}_p and $\dot{\beta}$ are represented in the forms (33) and (24a). For elastic-viscoplastic materials it is further assumed that $L_{p_{ij}}, \dot{\kappa}, \dot{\beta}_{ij}$ are specified by

$$L_{p_{ij}} = \Gamma \bar{L}_{p_{ij}}, \quad \dot{\kappa} = \Gamma \bar{K} - K, \quad \dot{\beta}_{ij} = \Gamma \bar{B}_{ij} - B_{ij}, \quad (36a, b, c)$$

where $\{\Gamma, \bar{L}_{p_{ij}}, \bar{K}, K, \bar{B}_{ij}, B_{ij}\}$ are functions of the variables \mathcal{V} only. In (36) the functions K and B_{ij} model the effects of thermal recovery of hardening, which are explicitly rate-dependent.

For rate-independent elastic-plastic response, it is assumed that Γ also depends linearly on the rates $\{D_{ij}, \dot{\theta}\}$. Furthermore, thermal recovery of hardening must vanish

$$K = 0, \quad B_{ij} = 0. \quad (37a, b)$$

Such a theory can be developed by introducing a yield surface in strain space (Naghdi and Trapp, 1975)

$$g(\mathcal{V}) \leq 0, \quad (38)$$

which separates the boundary between elastic and plastic response. Then, the function Γ can be determined by loading and unloading conditions. To this end, it is noted that

$$\mathbf{L}_m = \mathbf{D}_m + \mathbf{W}_m, \tag{39a}$$

$$\mathbf{D}_m = \frac{1}{2}(\mathbf{L}_m + \mathbf{L}_m^T) = \mathbf{D}_m^T = \mathbf{D} - \mathbf{D}_p, \tag{39b}$$

$$\mathbf{W}_m = \frac{1}{2}(\mathbf{L}_m - \mathbf{L}_m^T) = -\mathbf{W}_m^T = \mathbf{W} - \mathbf{W}_p, \tag{39c}$$

$$\mathbf{L}_p = \mathbf{D}_p + \mathbf{W}_p = \Gamma \mathbf{L}_p, \tag{39d}$$

$$\mathbf{D}_p = \frac{1}{2}(\mathbf{L}_p + \mathbf{L}_p^T) = \mathbf{D}_p^T = \Gamma \mathbf{D}_p, \tag{39e}$$

$$\mathbf{W}_p = \frac{1}{2}(\mathbf{L}_p - \mathbf{L}_p^T) = -\mathbf{W}_p^T = \Gamma \mathbf{W}_p, \tag{39f}$$

so that the rate of change of the metric m_{ij} can be written in the form

$$\dot{m}_{ij} = 2\mathbf{D}_m \cdot (\mathbf{m}_i \otimes \mathbf{m}_j) = 2\mathbf{D} \cdot (\mathbf{m}_i \otimes \mathbf{m}_j) - 2\mathbf{D}_p \cdot (\mathbf{m}_i \otimes \mathbf{m}_j). \tag{40}$$

Now, defining the functions

$$\hat{g} = 2 \frac{\partial g}{\partial m_{ij}} (\mathbf{m}_i \otimes \mathbf{m}_j) \cdot \mathbf{D} + \frac{\partial g}{\partial \theta} \dot{\theta}, \tag{41a}$$

$$\bar{g} = 2 \frac{\partial g}{\partial m_{ij}} (\mathbf{m}_i \otimes \mathbf{m}_j) \cdot \mathbf{D}_p - \frac{\partial g}{\partial \kappa} \bar{K} - \frac{\partial g}{\partial \beta_{ij}} \bar{B}_{ij}, \tag{41b}$$

the quantity \dot{g} may be written in the simple form

$$\dot{g} = \hat{g} - \Gamma \bar{g}, \tag{42}$$

and the function Γ may be determined by the loading conditions

$$\Gamma = 0 \quad \text{for elastic response} \quad (g < 0), \tag{43a}$$

$$\Gamma = 0 \quad \text{for unloading} \quad (g = 0 \text{ and } \hat{g} < 0), \tag{43b}$$

$$\Gamma = 0 \quad \text{for neutral loading} \quad (g = 0 \text{ and } \hat{g} = 0), \tag{43c}$$

$$\Gamma = \hat{g}/\bar{g} \quad \text{for loading} \quad (g = 0 \text{ and } \hat{g} > 0). \tag{43d}$$

Notice that (43d) is determined by the consistency condition which requires \dot{g} to vanish during loading.

To complete the constitutive description it is assumed that $\psi, \eta, \xi', \mathbf{T}, \mathbf{p}$ are functions of the forms

$$\psi = \psi(\mathcal{V}), \quad \eta = \eta(\mathcal{V}), \quad \xi' = \xi'(\mathcal{V}; \Gamma) \tag{44a, b, c}$$

$$\mathbf{T} = \mathbf{T}(\mathcal{V}, \mathbf{m}_i), \quad \mathbf{p} = \mathbf{p}(\mathcal{V}, \mathbf{g}, \mathbf{m}_i), \tag{44d, e}$$

where

$$\mathbf{p} = p_i(\mathcal{V}, g_j) \mathbf{m}^i, \quad g_j = \mathbf{g} \cdot \mathbf{m}_j, \tag{45a, b}$$

$$p_i^+ = p_i, \quad g_j^+ = g_j, \tag{45c, d}$$

and for simplicity the known result that $\{\psi, \eta, \mathbf{T}\}$ cannot depend on the temperature gradient \mathbf{g} has already been used. It is important to note that $\{\psi, \eta, \mathbf{T}\}$ are assumed to be independent of rates and that the function $p_i(\mathcal{V}, g_j)$ is an arbitrary function of its arguments. Now, with the help of eqns (36), (40) and (44), the reduced energy equation (17) may be rewritten in the form

$$\rho \left(\frac{\partial \psi}{\partial \theta} + \eta \right) \dot{\theta} + \left[2\rho \frac{\partial \psi}{\partial m_{ij}} (\mathbf{m}_i \otimes \mathbf{m}_j) - \mathbf{T} \right] \cdot \mathbf{D} + \rho \left[\theta \xi' - 2 \frac{\partial \psi}{\partial m_{ij}} (\mathbf{m}_i \otimes \mathbf{m}_j) \cdot \mathbf{D}_p + \frac{\partial \psi}{\partial \kappa} \dot{\kappa} + \frac{\partial \psi}{\partial \beta_{ij}} \dot{\beta}_{ij} \right] = 0. \quad (46)$$

For an elastic–viscoplastic material the coefficients of the rates $\{\dot{\theta}, \mathbf{D}\}$ and the last term in square brackets are independent of the rates $\{\dot{\theta}, \mathbf{D}\}$. Also the coefficient of \mathbf{D} is symmetric. Thus, for arbitrary but fixed values of \mathcal{V} , the rates $\{\dot{\theta}, \mathbf{D}\}$ may be chosen arbitrarily to deduce that

$$\eta = - \frac{\partial \psi}{\partial \theta}, \quad \mathbf{T} = 2\rho \frac{\partial \psi}{\partial m_{ij}} (\mathbf{m}_i \otimes \mathbf{m}_j), \quad (47a, b)$$

$$\rho \theta \xi' = \mathbf{T} \cdot \mathbf{D}_p - \rho \left[\frac{\partial \psi}{\partial \kappa} \dot{\kappa} + \frac{\partial \psi}{\partial \beta_{ij}} \dot{\beta}_{ij} \right], \quad (47c)$$

must hold for arbitrary thermomechanical processes. Alternatively, for an elastic–plastic material with a yield surface, either the values of \mathcal{V} are such that the response is elastic with vanishing values of $\{\mathbf{D}_p, \dot{\kappa}, \dot{\beta}_{ij}\}$ or the values of \mathcal{V} are such that the material is at the elastic–plastic boundary and the rates $\{\dot{\theta}, \mathbf{D}\}$ may be chosen such that the material unloads elastically, again with vanishing values of $\{\mathbf{D}_p, \dot{\kappa}, \dot{\beta}_{ij}\}$. In either case, the coefficients of the rates $\{\dot{\theta}, \mathbf{D}\}$ are independent of these rates so the results (47a, b) may be deduced. Furthermore, since the results (47a, b) are independent of rates they must hold for all thermomechanical processes including processes with nonvanishing values of $\{\mathbf{D}_p, \dot{\kappa}, \dot{\beta}_{ij}\}$. Consequently, substitution of (47a, b) into (46) yields the result (47c). Thus, the results (47a, b, c) hold for either elastic–viscoplastic or elastic–plastic materials of the type considered here.

The functional forms of the constitutive equations (36) and (44) must be suitably restricted so as to satisfy the three forms of the second law of thermodynamics (21a, b, c). In addition, it has been assumed [see eqn (9)] that $m_{ij} = \delta_{ij}$ whenever the present state is stress-free and at reference temperature θ_0 . In view of the result (47b), this means that the functional form of the Helmholtz free energy ψ must also be restricted so that

$$\frac{\partial \psi}{\partial m_{ij}} (\delta_{ij}, \theta_0, \kappa, \beta_{ij}) = 0, \quad (48)$$

for any possible values of κ and β_{ij} .

With regard to the additive separation (31) it is noted that \mathbf{L}_p characterizes the relaxation effects due to plastic deformation and \mathbf{L}_m characterizes the elastic part of the velocity gradient \mathbf{L} . The term \mathbf{L}_m is interpreted as the elastic part because in the absence of plastic relaxation effects ($\mathbf{L}_p = 0, \mathbf{L}_m = \mathbf{L}$) eqn (1) may be integrated to deduce that

$$\mathbf{m}_i = \mathbf{F} \mathbf{m}_i(0), \quad (49)$$

where $\mathbf{m}_i(0)$ are the values of \mathbf{m}_i measured in the reference configuration and \mathbf{F} is the deformation gradient between the reference and present configurations. Thus, for this special case, \mathbf{m}_i may be identified with material line elements. Furthermore, general anisotropic elastic response can be obtained by specifying vanishing values for $\mathbf{L}_p, \dot{\kappa}$ and $\dot{\beta}_{ij}$.

It follows from (4) that the ratio of the volume of the lattice in its present state to that in the RLS may be characterized by the dilatational measure J_m

$$J_m = m^{1/2}, \quad m = \det(m_{ij}), \quad (50a, b)$$

where it is noted that m is also equal to the determinant of the metric m_{ij} . Now, using the evolution equation (1) and the separation (31) it can be shown that

$$\frac{\dot{J}_m}{J_m} = \mathbf{L}_m \cdot \mathbf{I} = \mathbf{D} \cdot \mathbf{I} - \mathbf{D}_p \cdot \mathbf{I} = \frac{\dot{J}}{J} - \mathbf{D}_p \cdot \mathbf{I}, \quad (51)$$

where $J = \det \mathbf{F}$ is the relative volume between the present and reference configurations. For nonporous metals it is observed that the volume of the metal in a stress-free state at reference temperature θ_0 remains reasonably unaffected by prior relaxation effects of plasticity. This is usually interpreted to mean that plastic deformation is incompressible. Thus, within the present context, this restriction can be imposed by requiring the relaxation effects of plasticity to be isochoric so that (Van der Giessen, 1989, p. 20)

$$\mathbf{D}_p \cdot \mathbf{I} = 0. \quad (52)$$

Consequently, when (52) is satisfied then J_m is proportional to J .

5. ELASTICALLY ISOTROPIC RESPONSE

In view of the restriction (48) it follows that m_{ij} is a measure of elastic deformation which causes nonzero stress. For the discussion of a material which exhibits elastically isotropic response it is convenient to introduce a tensorial measure of deformation of the lattice from the RLS to the present state. To this end, the symmetric second-order tensor \mathbf{B}_m is defined by the formula

$$\mathbf{B}_m = \mathbf{m}_i \otimes \mathbf{m}_i, \quad (53)$$

which has the properties that

$$\mathbf{B}_m = \mathbf{I} \quad \text{for } m_{ij} = \delta_{ij}, \quad (54a)$$

$$\mathbf{B}_m^+ = \mathbf{Q} \mathbf{B}_m \mathbf{Q}^T. \quad (54b)$$

For an elastically isotropic material it is assumed that the Helmholtz free energy depends on m_{ij} only through the invariants of \mathbf{B}_m . Following the work of Flory (1961) for elastic response and Besseling (1968, p. 38) for elastic-plastic response the effects of dilatation and distortion are separated by defining the distortional part \mathbf{B}'_m of \mathbf{B}_m by the formulas

$$J_m = [\det \mathbf{B}_m]^{1/2}, \quad (55a)$$

$$\mathbf{B}'_m = J_m^{-2/3} \mathbf{B}_m, \quad \det(\mathbf{B}'_m) = 1. \quad (55b, c)$$

where the result (55a) connects the determinant of \mathbf{B}_m to the dilatational measure J_m defined in (50). Since \mathbf{B}'_m is a unimodular tensor† it has only two independent scalar invariants which may be written in the forms

$$\alpha_1 = \mathbf{B}'_m \cdot \mathbf{I} = J_m^{-2/3} m_{ii}, \quad (56a)$$

$$\alpha_2 = \mathbf{B}'_m \cdot \mathbf{B}'_m = J_m^{-4/3} m_{ij} m_{ij}. \quad (56b)$$

† The notation prime is not used in the sense of an operator so that \mathbf{B}'_m should not be confused as a deviatoric tensor even though later \mathbf{T}' will denote the deviatoric part of the stress tensor.

Thus, for elastically isotropic response it is assumed that the Helmholtz free energy ψ is a function of the form

$$\psi = \psi(\mathcal{U}), \tag{57}$$

where the variables \mathcal{U} are defined by

$$\mathcal{U} = \{J_m, \alpha_1, \alpha_2, \theta, \kappa, \beta_{ij}\}. \tag{58}$$

Now, with the help of the results

$$\frac{\partial J_m}{\partial m_{ij}} \mathbf{m}_i \otimes \mathbf{m}_j = \frac{1}{2} J_m m^{ij} \mathbf{m}_i \otimes \mathbf{m}_j = \frac{1}{2} J_m \mathbf{I}, \tag{59a}$$

$$\frac{\partial \alpha_1}{\partial m_{ij}} \mathbf{m}_i \otimes \mathbf{m}_j = J_m^{-2/3} [\delta_{ij} - \frac{1}{3} (\mathbf{B}_m \cdot \mathbf{I}) m^{ij}] \mathbf{m}_i \otimes \mathbf{m}_j = [\mathbf{B}'_m - \frac{1}{3} (\mathbf{B}'_m \cdot \mathbf{I}) \mathbf{I}], \tag{59b}$$

$$\frac{\partial \alpha_2}{\partial m_{ij}} \mathbf{m}_i \otimes \mathbf{m}_j = 2 J_m^{-4/3} [m_{ij} - \frac{1}{3} (\mathbf{B}_m^2 \cdot \mathbf{I}) m^{ij}] \mathbf{m}_i \otimes \mathbf{m}_j = 2 [\mathbf{B}'_m{}^2 - \frac{1}{3} (\mathbf{B}'_m{}^2 \cdot \mathbf{I}) \mathbf{I}], \tag{59c}$$

together with the restriction (47b) it may be shown that the pressure p and the deviatoric part \mathbf{T}' of the Cauchy stress are given by the formulas

$$\mathbf{T} = -p \mathbf{I} + \mathbf{T}', \quad \mathbf{T}' \cdot \mathbf{I} = 0, \tag{60a, b}$$

$$p = -\rho J_m \frac{\partial \psi}{\partial J_m}, \tag{60c}$$

$$\mathbf{T}' = 2\rho \frac{\partial \psi}{\partial \alpha_1} [\mathbf{B}'_m - \frac{1}{3} (\mathbf{B}'_m \cdot \mathbf{I}) \mathbf{I}] + 4\rho \frac{\partial \psi}{\partial \alpha_2} [\mathbf{B}'_m{}^2 - \frac{1}{3} (\mathbf{B}'_m{}^2 \cdot \mathbf{I}) \mathbf{I}]. \tag{60d}$$

Further, with reference to the restriction (48) it is noticed from (60d) that the deviatoric stress \mathbf{T}' vanishes when $\mathbf{B}'_m = \mathbf{I}$ even when the temperature is not equal to the reference temperature. This means that the restriction (48) will be satisfied if ψ is restricted by the condition

$$\frac{\partial \psi}{\partial J_m} = 0 \quad \text{for } J_m = 1 \quad \text{and} \quad \theta = \theta_0. \tag{61}$$

It is of interest to note that by using (1), the tensor \mathbf{B}'_m can be calculated directly by integrating an equation of the form

$$\dot{\mathbf{B}}'_m = \mathbf{L}_m \mathbf{B}'_m + \mathbf{B}'_m \mathbf{L}_m^T - \frac{2}{3} (\mathbf{D}_m \cdot \mathbf{I}) \mathbf{B}'_m. \tag{62}$$

Furthermore, by using the separation (31) and the plastic incompressibility condition (52) (62) may be rewritten in the alternative form

$$\dot{\mathbf{B}}'_m = [\mathbf{L} \mathbf{B}'_m + \mathbf{B}'_m \mathbf{L}^T - \frac{2}{3} (\mathbf{D} \cdot \mathbf{I}) \mathbf{B}'_m] - [\mathbf{L}_p \mathbf{B}'_m + \mathbf{B}'_m \mathbf{L}_p^T]. \tag{63}$$

It also follows that

$$\dot{\alpha}_1 = \dot{\mathbf{B}}'_m \cdot \mathbf{I} = 2 [\mathbf{B}'_m \cdot \mathbf{D} - \frac{1}{3} (\mathbf{D} \cdot \mathbf{I}) (\mathbf{B}'_m \cdot \mathbf{I})] - 2 [\mathbf{B}'_m \cdot \mathbf{D}_p], \tag{64a}$$

$$\dot{\alpha}_2 = 2 \dot{\mathbf{B}}'_m \cdot \mathbf{B}'_m = 2 [\mathbf{B}'_m{}^2 \cdot \mathbf{D} - \frac{1}{3} (\mathbf{D} \cdot \mathbf{I}) (\mathbf{B}'_m{}^2 \cdot \mathbf{I})] - 2 [\mathbf{B}'_m{}^2 \cdot \mathbf{D}_p]. \tag{64b}$$

This means that even though the invariants α_1 and α_2 are not influenced by the plastic spin \mathbf{W}_p , the direction of \mathbf{B}'_m and hence the direction of stress \mathbf{T}' are influenced by \mathbf{W}_p .

Although the stress response associated with the functional form (57) is elastically isotropic, the plastic response may retain or develop directional dependence. This means that the functional forms for the evolution equations (36) remain general. However, as a special case, it may be of interest to specify the relaxation effects of plasticity on the evolution of \mathbf{B}'_m directly by taking \mathbf{L}_p to be a solution† of the equation

$$\mathbf{L}_p \mathbf{B}'_m + \mathbf{B}'_m \mathbf{L}_p^T = \Gamma \mathbf{A}, \quad (65)$$

so that (63) may be rewritten in the form

$$\dot{\mathbf{B}}'_m = [\mathbf{L} \mathbf{B}'_m + \mathbf{B}'_m \mathbf{L}^T - \frac{2}{3} (\mathbf{D} \cdot \mathbf{I}) \mathbf{B}'_m] - \Gamma \mathbf{A}. \quad (66)$$

In (65) and (66) the tensor \mathbf{A} requires a constitutive equation, which in view of the plastic incompressibility condition (52) must satisfy the restriction

$$\mathbf{A} \cdot \mathbf{B}'_m{}^{-1} = 0. \quad (67)$$

Assuming that \mathbf{A} is a function of \mathbf{B}'_m and the variables \mathcal{U} only, it follows from invariance under SRBM that \mathbf{A} must be an isotropic function of \mathbf{B}'_m which may be represented in the general form

$$\mathbf{A} = a_1(\mathcal{U}) \left[\mathbf{B}'_m - \left(\frac{3}{\mathbf{B}'_m{}^{-1} \cdot \mathbf{I}} \right) \mathbf{I} \right] + a_2(\mathcal{U}) \left[\mathbf{B}'_m{}^2 - \left(\frac{\mathbf{B}'_m \cdot \mathbf{I}}{3} \right) \mathbf{B}'_m \right]. \quad (68)$$

This means that as far as the calculation of \mathbf{B}'_m is concerned it is not necessary to specify \mathbf{L}_p explicitly because it is enough to specify \mathbf{A} . In this regard, it is noted that constitutive equations of the type (66) and (68) have been considered by Leonov (1976).

Using the definition (5a) and the evolution equation (1) it can also be shown that

$$\dot{\mathbf{m}}^i = -\mathbf{L}_m^T \mathbf{m}^i, \quad (69)$$

so that with the help of (24) the evolution equation (36c) may be rewritten in the form

$$\dot{\boldsymbol{\beta}} = -\mathbf{L}_m^T \boldsymbol{\beta} - \boldsymbol{\beta} \mathbf{L}_m + \Gamma \mathbf{N} - \mathbf{B}, \quad (70)$$

where the tensors \mathbf{N} and \mathbf{B} are defined by

$$\mathbf{N} = N_{ij} \mathbf{m}^i \otimes \mathbf{m}^j, \quad \mathbf{B} = B_{ij} \mathbf{m}^i \otimes \mathbf{m}^j. \quad (71a, b)$$

Now, using the representations (31) and (36a), eqn (70) may be rewritten in the form

$$\dot{\boldsymbol{\beta}} = -\mathbf{L}^T \boldsymbol{\beta} - \boldsymbol{\beta} \mathbf{L} + \Gamma \mathbf{N} - \mathbf{B}, \quad \mathbf{N} = \bar{\mathbf{B}} + \mathbf{L}_p^T \boldsymbol{\beta} + \boldsymbol{\beta} \mathbf{L}_p. \quad (72a, b)$$

Thus, as a special case it could be assumed that the tensors \mathbf{N} and \mathbf{B} are isotropic functions of \mathbf{B}'_m and $\boldsymbol{\beta}$.

† It can be shown that \mathbf{L}_p cannot be uniquely determined by eqn (65) unless it is a symmetric tensor.

6. SMALL ELASTIC DEFORMATIONS

For small elastic deformations it is assumed that the metric m_{ij} may be expressed in the form

$$m_{ij} = \delta_{ij} + 2\varepsilon_{ij}, \quad (73)$$

where ε_{ij} is a symmetric strain tensor which is of order ε relative to unity. In the following expressions, terms of order ε^2 are neglected consistently relative to terms of order ε . Consequently, using (6a), (7a) and (73) it may be shown that

$$\mathbf{m}_i = (\delta_{im} + \varepsilon_{im})\mathbf{a}_m, \quad \mathbf{a}_i = (\delta_{im} - \varepsilon_{im})\mathbf{m}_m, \quad (74a, b)$$

where \mathbf{a}_i are the orthogonal vectors defined by (7b). Next, with the help of (40) and (74) one obtains

$$\dot{\varepsilon}_{ij} = (\mathbf{D} - \mathbf{D}_p) \cdot (\mathbf{a}_i \otimes \mathbf{a}_j), \quad (75)$$

so that differentiation of (74b) and use of (1), (31), (39) and (75) yields

$$\dot{\mathbf{a}}_i = (\mathbf{W} - \mathbf{W}_p)\mathbf{a}_i. \quad (76)$$

Furthermore, in view of the results (11a, c) it follows that under SRBM ε_{ij} transforms by

$$\varepsilon_{ij}^+ = \varepsilon_{ij}, \quad (77)$$

and \mathbf{a}_i continues to transform by (11c). Consequently, for small elastic deformations, \mathbf{a}_i is an orthonormal triad related to specified crystallographic directions which is determined by integrating (76), and ε_{ij} is the elastic strain which is determined by integrating (75).

In order to consider the more special case of rigid-plastic response it is assumed that the constitutive equation for \mathbf{D}_p can be inverted to obtain an expression for m_{ij} (or its deviatoric part) in terms of the components $[\mathbf{D}_p \cdot (\mathbf{a}_i \otimes \mathbf{a}_j)]$. Then, with the help of these values of m_{ij} , eqns (74), (75) and the constitutive equation (47b), the stress \mathbf{T} can be written as a function of \mathbf{D}_p , \mathbf{a}_i and possibly a constraint response for the pressure of an incompressible material. Finally, in the rigid-plastic limit $\dot{\varepsilon}_{ij}$ is negligible in (75) so that \mathbf{D}_p can be approximated by \mathbf{D} .

7. DISCUSSION

In the previous sections a general theoretical structure for modeling anisotropic elastic-plastic material response has been developed which is independent of the choice of the reference configuration from which total strain is measured. Specifically, the theory requires specification of functional forms for: the Helmholtz free energy (44a); the entropy flux (44e); the relaxation effects of plasticity (36a); the evolution equations of hardening (36b, c). Then the entropy, Cauchy stress and rate of entropy production are determined by the expressions (47) and (16). In addition, the restrictions (21) due to the second law of thermodynamics and the physical restriction (48) must be satisfied. Next, using the result (31) the evolution equations (1) and (36b, c) for \mathbf{m}_i , κ and β_{ij} may be integrated to deduce the response to any specified thermomechanical process.

Within the context of the present development it has been proved [see the discussion of eqn (31)] that the velocity gradient separates additively into a part \mathbf{L}_m which controls the evolution of elastic deformation and a part \mathbf{L}_p which controls the relaxation effects of plasticity. An interesting consequence of this separation is that when the Helmholtz free energy is independent of the hardening variables, the rate of plastic dissipation reduces to the usual expression for the rate of plastic work, since (21c) and (47c) yield

$$\rho\theta\xi' = \mathbf{T} \cdot \mathbf{D}_p \geq 0. \quad (78)$$

In order to model the orientation and the elastic deformation of the average atomic lattice a vector triad \mathbf{m}_i has been introduced which is determined by the present physical state of the material. The metric m_{ij} (5b) determines the elastic deformation of the lattice relative to the Reference Lattice State (RLS) and the orthonormal vectors \mathbf{a}_i (7b) determine the present orientation of the lattice. In this sense, material anisotropies may be referred to the directions \mathbf{a}_i which are determined by the current physical state of the material. An important physical feature of the present development is that the quantities $\{\mathbf{m}_i, \kappa, \beta_{ij}\}$ are, in principle, measurable in the present state of the material. This means that the initial values of $\{\mathbf{m}_i, \kappa, \beta_{ij}\}$ are measurable so the evolution equations for the rates of $\{\mathbf{m}_i, \kappa, \beta_{ij}\}$ can be integrated without ambiguity.

To further elaborate it is noted that the forms of the constitutive equations are intimately related to the specification of \mathbf{m}_i in the present state. For example, for the simple case of a single atomic lattice discussed in the beginning of Section 2, the vectors \mathbf{m}_i are related to the directions \mathbf{e}_i by the formula (3). This means that \mathbf{m}_i will depend on the specific choice used to define the lattice directions \mathbf{D}_i relative to the fixed vectors \mathbf{e}_i . Consequently, the functional form (44a) for the Helmholtz free energy ψ will also depend on this choice. This merely means that in order to characterize the anisotropic response of a material through a specific functional form for ψ it is necessary to also specify the reference frame (relative to identifiable directions in the present material state) with respect to which the functional form was evaluated. This is of course well known for fiber reinforced composite materials where it is natural to use the fiber directions as a reference for modeling anisotropic elastic response.

For thermoelastic materials it is common to specify the Helmholtz free energy in the form

$$\psi = \psi(\mathbf{C}, \theta) \quad (79)$$

which has the physical problem (P1) discussed in the Introduction because \mathbf{C} and the functional form for ψ depend explicitly on the specification of the reference configuration. In contrast, specialization of (44a) for elastic response suggests that

$$\psi = \psi(m_{ij}, \theta), \quad (80)$$

which has the physical features that the functional form for ψ is independent of the choice of the reference configuration and that it depends explicitly on material directions, characterized by \mathbf{m}_i , which are measurable in the present material state. Any material symmetries which cause nonuniqueness of the vectors \mathbf{m}_i must be accompanied by complementary restrictions on the constitutive equations that ensure the material response is unaffected by this nonuniqueness. This discussion suggests that even for elastic materials, this approach seems to clarify the explicit dependence of anisotropy on identifiable material directions in the present state. Further in this regard, it is recalled that for the simplest case of elastic response without plastic relaxation effects [see eqn (49)], the vectors \mathbf{m}_i can be related to tangent vectors associated with convected coordinates along the \mathbf{e}_i directions in the RLS. Then the material anisotropies can be defined relative to these convected coordinates and the functional form (80) becomes similar to that given by eqn (2.3.8) of Green and Zerna (1968, p. 63) with m_{ij} playing the role of the metric.

In order to discuss the relationship of the present theory with others for elastic-plastic response it is recalled that the theory proposed by Green and Naghdi (1965) is equivalent to assuming the existence of a symmetric positive definite plastic deformation tensor \mathbf{C}_p that is determined by integrating an evolution equation of the form

$$\dot{\mathbf{C}}_p = \mathbf{A}_p, \quad (81)$$

where \mathbf{A}_p requires a constitutive equation. Then, the elastic response of the material is specified by taking

$$\psi = \psi(\mathbf{C}, \mathbf{C}_p, \theta), \quad (82)$$

where hardening variables which are usually included in (82) are not exhibited explicitly here because they are not particularly relevant to the present discussion.

Green and Naghdi (1965, footnote, p. 260) stated that for full generality the plastic deformation tensor should be nonsymmetric. Within this context it is possible to define a nonsingular nonsymmetric tensor \mathbf{F}_p by the evolution equation

$$\dot{\mathbf{F}}_p = \mathbf{A}_p \mathbf{F}_p, \quad (83)$$

where \mathbf{A}_p requires a constitutive equation. In particular, it is noted that the invariance properties of \mathbf{F}_p under SRBM are determined by the invariance properties of \mathbf{A}_p . Thus, for example, if \mathbf{A}_p is trivially invariant under SRBM then \mathbf{F}_p will also be trivially invariant under SRBM. Using \mathbf{F}_p the elastic response of the material can be determined by specifying the Helmholtz free energy in the form

$$\psi = \psi(\mathbf{C}, \mathbf{F}_p, \theta), \quad (84)$$

instead of the form (82). A particular example of a constitutive equation for \mathbf{A}_p associated with crystal plasticity has been suggested by Rice (1971).

The formulations using either (82) or (84) suffer from the physical problem (P1) discussed in the Introduction because the Helmholtz free energy depends explicitly on the choice of the reference configuration through the tensor \mathbf{C} . Obviously, this problem persists even for elastic response with constant values of \mathbf{C}_p and \mathbf{F}_p , which has been alluded to by Onat (1982, p. 244) with reference to the deformation gradient \mathbf{F} . Moreover, since \mathbf{C}_p and \mathbf{F}_p are kinetic and not kinematic quantities it is necessary to specify how they transform under changes of the reference configuration in order to explore the influences of these changes on the functional forms (82) and (84). Also, assuming that \mathbf{C}_p and \mathbf{F}_p are measures of plastic deformation from the reference configuration, it follows that the formulations using either (82) or (84) suffer from the physical problem (P2) because the values of \mathbf{C}_p and \mathbf{F}_p cannot be measured given the present state of the material alone.

Another approach, which has been used by a number of authors (Lee and Liu, 1967; Lee, 1969; Rice, 1971; Mandel, 1973; Dafalias, 1985; Loret, 1983), is to assume that the total deformation gradient separates multiplicatively into an elastic part \mathbf{F}_e and a plastic part \mathbf{F}_p , such that

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p. \quad (85)$$

In (85) the tensor \mathbf{F}_p is presumed to describe the plastic deformation of the line element $d\mathbf{X}$ in the reference configuration into the line element $d\mathbf{y}$ in an intermediate unstressed configuration at reference temperature θ_0 , and the tensor \mathbf{F}_e is presumed to describe the elastic deformation of $d\mathbf{y}$ into the line element $d\mathbf{x}$ in the present configuration such that

$$d\mathbf{x} = \mathbf{F}_e d\mathbf{y}, \quad d\mathbf{y} = \mathbf{F}_p d\mathbf{X}. \quad (86a, b)$$

It is well known that for inhomogeneous deformations, \mathbf{F}_e and \mathbf{F}_p are not integrable, whereas \mathbf{F} is always integrable in terms of a displacement field.

If the plastic deformation \mathbf{F}_p is determined by an evolution equation of the type (83) then (85) is merely a definition of the tensor \mathbf{F}_e since

$$\mathbf{F}_e = \mathbf{F}\mathbf{F}_p^{-1}. \quad (87)$$

In this regard it follows that the invariance properties (under SRBM) of \mathbf{F}_e are determined by the invariance properties of \mathbf{F} and \mathbf{F}_p . However, if \mathbf{F}_p is not determined by an evolution equation, then the separation (85) is not unique and the proper definition and invariance properties (under SRBM) of \mathbf{F}_e and \mathbf{F}_p in (85) are controversial [see Naghdi (1990) Sections 4A and 4C]. Setting this point aside it is possible to define the symmetric elastic deformation tensor \mathbf{C}_e by

$$\mathbf{C}_e = \mathbf{F}_e^T \mathbf{F}_e. \quad (88)$$

One of the main motivations for defining \mathbf{C}_e is the tacit assumption that the Helmholtz free energy ψ for an elastic–plastic material depends on total deformation \mathbf{F} and plastic deformation \mathbf{F}_p only through the elastic deformation \mathbf{C}_e so that ψ has a similar form to (79) for an elastic material

$$\psi = \psi(\mathbf{C}_e, \theta). \quad (89)$$

Still another approach, which has been used by Eckart (1948), Besseling (1968), and Leonov (1976), is to propose a constitutive equation for the evolution of elastic deformation directly without introducing a plastic deformation tensor. For example, Eckart (1948) and Leonov (1976) independently introduced an evolution equation for the rate of change of the symmetric tensor $\mathbf{B}_e = \mathbf{F}_e \mathbf{F}_e^T$. In their formulations (Eckart, 1948; Leonov, 1976), the tensor \mathbf{B}_e had invariance properties under SRBM which only allowed for the characterization of elastically isotropic material response using the functional form (89) with \mathbf{C}_e replaced by \mathbf{B}_e . In contrast, Besseling's (1968) formulation proposed an evolution for the nonsingular nonsymmetric tensor \mathbf{F}_e of the form

$$\dot{\mathbf{F}}_e = \mathbf{L}_e \mathbf{F}_e, \quad (90)$$

which allowed the development of general anisotropic constitutive equations using (89) with \mathbf{C}_e defined by (88). In this formulation the tensor \mathbf{L}_e requires a constitutive equation which includes the relaxation effects of plasticity without introducing \mathbf{F}_p explicitly. Again, it is noted that the invariance properties of \mathbf{F}_e under SRBM are determined by the invariance properties of \mathbf{L}_e .

Within the context of the interpretation (86) it follows that \mathbf{F}_p is influenced by changes in both the reference and intermediate configurations and \mathbf{F}_e is influenced by changes in both the intermediate and present configurations. Thus, the formulation associated with (86) which uses the functional form (89) suffers from both of the physical problems (P1) and (P2) discussed in the Introduction. Moreover, within the context of the formulation of Besseling (1968) the line element dy in the natural reference state changes with time due to plastic deformation in a similar manner to the changes of dy in (86c) due to plastic deformations. Thus, the formulation associated with (90) which uses the functional form (89) suffers from the physical problems (P1) because the initial value of \mathbf{F}_e cannot be determined by knowledge of the present state of the material alone.

Mandel's (1973) physical description of specific directions in the isoclinic intermediate configuration is similar to the description by Besseling (1968) of directions in the natural reference state. As previously noted, the notion used here that the average atomic lattice can be represented by a triad of vectors \mathbf{m}_i is similar to the notion used by Mandel (1973) to represent the atomic orientation of the relaxed configuration with a triad of directors. However, the theory proposed by Mandel (1973) uses the multiplicative separation (85) so that it suffers from both of the physical problems (P1) and (P2). Moreover, Mandel's theory assumes that the directors remain orthonormal vectors that cease to rotate when plastic deformation ceases. In contrast, the present theory differs from that of Mandel

(1973) in three main ways: (a) it is independent of the choice of the reference configuration; (b) it is developed without introducing a definition for a plastic deformation tensor and without assuming that the total deformation gradient can be represented as the product of elastic and plastic deformation tensors (85); (c) the vectors \mathbf{m}_i represent the present state of the material and therefore rotate and deform even when plastic relaxation effects are absent. Also, the vectors \mathbf{m}_i characterize the present state of the microstructure and are not directly related to either of the line elements $d\mathbf{X}$ or $d\mathbf{y}$ or $d\mathbf{x}$. In this regard, the use of the vectors \mathbf{m}_i is consistent with the notions proposed by Onat (1968) which emphasize that state variables should be measurable in the present state. Consequently, the present theory does not suffer from either of the physical problems (P1) or (P2).

The need for specifying a constitutive equation for plastic spin \mathbf{W}_p is apparent in the work of Besseling (1968) which focused on the relaxation effects of plasticity as well as in the work of Kratochvil (1971, 1973) and Mandel (1973). Also, a specific form for \mathbf{W}_p associated with crystal plasticity can be obtained using the work of Rice (1971) or Asaro and Needleman (1985). Loret (1983) and Dafalias (1985) proposed specific continuum constitutive equations for plastic spin which were mainly motivated by the desire to find a better objective rate for hypoelastic formulations of plasticity theory. This work was continued by Dafalias in a number of papers that are referred to in Dafalias (1987, 1988). In particular, Dafalias (1985) and Loret (1983) assumed that \mathbf{W}_p is a function of the deviatoric stress \mathbf{T}' and a backstress tensor $\boldsymbol{\alpha}$ which transforms under SRBM by a transformation of the type (22c) so that

$$\mathbf{W}_p = \mathbf{W}_p(\mathbf{T}', \boldsymbol{\alpha}). \quad (91)$$

Recognizing that invariance under SRBM requires \mathbf{W}_p to be an isotropic function of its arguments, they used a representation theorem for isotropic functions to deduce the simplest form for \mathbf{W}_p . Alternatively, it is possible to develop a more general form than (91) by defining $\bar{\boldsymbol{\alpha}}$ as elastically embedded relative to $\boldsymbol{\alpha}$ such that

$$\boldsymbol{\alpha} = \mathbf{F}_e \bar{\boldsymbol{\alpha}} \mathbf{F}_e^T, \quad (92)$$

and replacing $\boldsymbol{\alpha}$ in (91) by $\bar{\boldsymbol{\alpha}}$. However, the resulting constitutive equation suffers from the physical problems (P1) and (P2) since \mathbf{F}_e is influenced by changes in the intermediate configuration which is directly related to plastic deformation from the reference configuration.

To emphasize the more general nature of the present formulation it is noted that if the vectors \mathbf{m}_i are included as independent variables in (91), then \mathbf{W}_p admits the representation

$$\mathbf{W}_p = W_{pij}[\mathbf{T}' \cdot (\mathbf{m}_i \otimes \mathbf{m}_j), \boldsymbol{\alpha} \cdot (\mathbf{m}_i \otimes \mathbf{m}_j), m_{rs}] \mathbf{m}^i \otimes \mathbf{m}^j, \quad (93)$$

where W_{pij} is an *arbitrary* skew-symmetric (in the indices i, j) function of its arguments. This is similar to the development of the form for \mathbf{L}_p in eqn (36a). It is also similar to the spin of the reference triad used by Raniecki and Mroz (1990) to characterize texture in rigid-plastic solids.

Sometimes material anisotropy is characterized with respect to orientational tensors instead of with respect to a specific vector triad. For example, one can examine the discussion of Dafalias (1987) of the relationship between the work of Mandel (1973) and that of Onat (1982). More specifically, Loret and Dafalias (1992) have formulated a constitutive equation for plastic spin in terms of purely orientational structure variables associated with a set of orthonormal vectors. However, Loret and Dafalias (1992) do not allow for the generality of a form like (93). Further in this regard, it is mentioned that alternatively one could assume that \mathbf{L}_p is a function of the form

$$\mathbf{L}_p = \mathbf{L}_p(\mathbf{m}_i, \theta, \kappa, \beta; \mathbf{D}, \dot{\theta}). \quad (94)$$

Then, by requiring \mathbf{L}_p to be an isotropic function of its arguments it is possible to recover the general form (33).

Next, it is mentioned that the functional forms of the Helmholtz free energy and the relaxation effects of plasticity are in general influenced by changing values of κ and β_{ij} . This means that the theory can model changes in elastic and plastic properties due to the evolution of texture. In particular, the triad \mathbf{m}_i can rotate and orient itself with directions defined by the deformation history [this will be discussed in more detail in the companion paper Rubin (1994)]. In this sense, the conclusion of Van der Giessen (1989) that the work of Besseling (1968) cannot model hardening effects or texturing effects seems to be limited to the assumption that the Helmholtz free energy and the plastic relaxation tensor do not depend on hardening variables like κ and β_{ij} . However, it should be mentioned that the present work assumes that the RLS is unaffected by material processing. Within this context, changes in the RLS may be considered to be a phase transition (a change from one material to another) which has not been modeled explicitly.

In summary, the general theoretical structure discussed in this paper represents a reasonably simple, physically based model for elastic–plastic materials. Within this context, the outstanding problem remains the specification of physically meaningful constitutive equations for the evolution equation (1) for the triad \mathbf{m}_i , and the evolution equations (36b,c) for the hardening variables. To this end, in a companion paper (Rubin, 1994), specific constitutive equations are discussed for a class of materials which are elastically isotropic but which exhibit directional properties for plastic relaxation effects.

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