

A principle of virtual work for combined electrostatic and mechanical loading of materials

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Abstract

The equations governing mechanics and electrostatics are formulated for a system in which the material deformations and electrostatic polarizations are arbitrary. A mechanical/electrostatic energy balance is formulated for this situation in terms of the electric enthalpy, in which the electric potential and the electric field are the independent variables, and charge and electric displacement, respectively, are the conjugate thermodynamic forces. This energy statement is presented in the form of a principle of virtual work (PVW), in which external virtual work is equated to internal virtual work. The resulting expression involves an internal material virtual work in which (1) material polarization is work-conjugate to increments of electric field, and (2) a combination of Cauchy stress, Maxwell stress and a product of polarization and electric field is work-conjugate to increments of strain. This PVW is valid for all material types, including those that are conservative and those that are dissipative. Such a virtual work expression is the basis for a rigorous formulation of a finite element method for problems involving the deformation and electrostatic charging of materials, including electroactive polymers and switchable ferroelectrics. The internal virtual work expression is used to develop the structure of conservative constitutive laws governing, for example, electroactive elastomers and piezoelectric materials, thereby determining the form of the Maxwell or electrostatic stress. It is shown that the Maxwell or electrostatic stress has a form fully constrained by the constitutive law and cannot be chosen independently of it. The structure of constitutive laws for dissipative materials, such as viscoelastic electroactive polymers and switchable ferroelectrics, is similarly determined, and it is shown that the Maxwell or electrostatic stress for these materials is identical to that for a material having the same conservative response when the dissipative processes in the material are shut off. The form of the internal virtual work is used further to develop the structure of dissipative constitutive laws controlled by rearrangement of material internal variables.

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1. Introduction

The principle of virtual work (PVW) provides an important framework that is used to generate exact and approximate solutions for problems in mechanics and electrostatics, and is the basis for the finite element method. A PVW for problems of simultaneous electrostatic and mechanical loading, with material interactions between the resulting strain and polarization, is needed for analyzing the response of switchable

ferroelectrics and electroactive polymers, among other materials. Ferroelectrics undergo dissipative domain switching driven by both electrostatic and mechanical loads [1]. Electroactive polymers are subject to high electric fields, and respond with a large actuation strain. In addition, electrostatic systems generally couple electrically to the aether in which they are located and force interactions occur through it. Thus, the requisite PVW must allow for dissipative processes in materials, should be valid for large deformations, and ought to take account of action at a distance through such features as the Maxwell stress [2]. In contrast, existing treatments [3–5] lack the requisite generality. This paper presents such a PVW that is valid under the very general conditions just described. It is based on the

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displacement and the electric potential as the independent variables, and is suitable as the foundation of a finite element method in which such parameters are taken to be the nodal variables. The approach that we take is consistent with, and repeats some aspects of, the treatments of the electrostatics of deformable bodies that are recognized as classical, and that are generally regarded as the foundations of its analysis. An incomplete list of these publications comprises the works of Toupin [6], Truesdell and Toupin [7], Eringen [8], Tiersten [9], Pao [10], Hutter and van de Ven [11], Maugin [12], Eringen and Maugin [13], Tiersten [14] and Kovetz [15]. In addition, recent presentations of the topic include the paper of Dorfmann and Ogden [16]. The basis of our developments presented below is to be found in the above papers and treatises. Nevertheless we believe our presentation provides a useful contribution that forms the foundation of finite element formulations for the analysis of a wide variety of electrostatically stimulated deformable materials, whether conservative or dissipative. In this regard, we have found no previous publication that provides our statement of the PVW. In addition, we give the structure of conservative and dissipative constitutive laws for electroactive materials, and use it to determine the associated form of the Maxwell or electrostatic stress, inclusive of electrostrictive effects and consistent with such constitutive laws. We are not aware of any previous paper giving such a prescription for the Maxwell or electrostatic stress for a dissipative material such as a switching ferroelectric or a viscoelastic electroactive polymer. In addition, a foundation for an irreversible constitutive law for dissipative electroactive materials, dependent on internal variables, is formulated, based on considerations of Gibbs free energy deduced from the PVW. Furthermore, we assert that our formulation of the electrostatics of a deformable body is more suitable as a starting point for finite element formulations, both conservative and dissipative, than treatments that have been presented previously, because it provides the appropriate PVW in the most flexible format in which no prior assumption is made regarding the form of the Maxwell or electrostatic stresses, or their separability from the electrostrictive stresses. In addition, the PVW we provide fits readily into the framework that is most widely used in the finite element field for large deformation problems [17,18].

2. Basic formulation

This section repeats closely the foundations from a previous paper [5] that was confined to conservative materials and provided work statements with displacement and charge configuration as the independent variables. Instead, this paper will provide a PVW that is completely general, and will provide it with displacement and electric potential as the independent variables, so making it usable as the starting point for finite element formulations that utilize those parameters as the independent variables. For convenience the outline of the basic equations in common with the previous work will be given, since it provides the strong formulation of the problem upon which the weak, PVW, form is developed.

Consider a system consisting of dielectric materials, perfect conductors and free space, without any implication that the dielectricity is conservative or linear. In the current configuration, the system occupies the volume V . The perimeter of the system plus interfaces within it are designated S in the current configuration. The internal interfaces separate the dielectric materials, the conductors and free space from each other. In addition, sectors of dielectric with homogeneous or heterogeneous properties may be separated by surfaces included within S , as may sectors of free space.

Let the free charge per unit volume within V be $q(x_i, t)$ where x_i is the position of material points in the current configuration and t is time. Free charge may be placed in free space, in which case x_i is used to designate the position of the points occupied by free space in the current configuration. Furthermore, let $\omega(x_i, t)$ be the free charge per unit area on the surfaces S and define $\phi(x_i, t)$ to be the electrical potential everywhere within the system such that it is continuous everywhere in space. Note that we will consider only the electrostatic limit so that t plays the role of a load parameter as far as the electrical variables are concerned and no attempt will be made to explore Maxwell's equations relevant to the electrodynamic limit. On the other hand, time may have a real meaning as far as the deformation of material is concerned, as may be the case in strain-rate dependent response or in the acoustic limit where inertia must be included in the balance laws. Further variables to be considered in the PVW are the velocity $v_i(x_i, t)$ of material points, the surface traction $T_i(x_i, t)$ defined as the force per unit area acting on S and $b_i(x_i, t)$, which is the body force per unit volume acting at points in V . Note that the surface traction T_i and the body force b_i arise from sources other than electrical effects and therefore, do not represent the influence of charges interacting at a distance or electrical fields exerting forces on charges. The surface traction T_i and the body force b_i and any equivalent quantity defined in the current state will be designated mechanical.

Consider the physical laws governing the electromechanical fields in the material. In the quasi-static limit, Maxwell's laws state that the electric field must be curl-free and Gauss's law states that the divergence of the electric displacement must be equal to the volume density of free charge. Therefore, for the electric field, E_i , and the electric displacement, D_i ,

$$\varepsilon_{ijk} \frac{\partial E_j}{\partial x_k} = 0 \Rightarrow E_i = -\frac{\partial \phi}{\partial x_i}, \quad (1)$$

$$\frac{\partial D_i}{\partial x_i} = q \quad \text{in } V, \quad (2)$$

$$n_i \| D_i \| = \omega \quad \text{on } S. \quad (3)$$

Here, n_i are the Cartesian components of the unit normal to the surface S pointing from the “−” side of the surface out towards the “+” side, and ε_{ijk} are the components of the permutation symbol. The notation $\| \|$ represents the difference or jump in

the included quantity across the surface S such that

$$\|D_i\| = D_i^+ - D_i^- \tag{4}$$

Note that finite regions V that exclude charges lying outside them may be considered to be bound by the exterior portion of S , with D_i^+ set to zero beyond there, and a virtual value of ω chosen on the exterior perimeter to represent the electrostatic actions of all the charge in the excluded region; *i.e.* the boundary condition on the exterior perimeter of the region V to be considered, in the form of a virtual free charge and the true electric potential, represents the electrostatic influence of the excluded region on the retained segment, much in the way that surface tractions and displacements on the perimeter of a free body isolated from a larger body represent the mechanical action of the excluded material on that free body.

The electric displacement can be decomposed into two parts such that

$$D_i = \kappa_0 E_i + P_i, \tag{5}$$

where κ_0 is the dielectric permittivity of free space and P_i are the Cartesian components of the material polarization.

Conservation of mass implies that for a given material volume

$$\frac{d}{dt} \int_V \rho \, dV = 0 \Rightarrow \frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_i} = 0, \tag{6}$$

where $\rho(x_i, t)$ is the mass density of the material. The principles of conservation of linear and angular momentum are stated as

$$\int_V (b_i + b_i^E) \, dV + \int_S (T_i + T_i^E) \, dS = \frac{d}{dt} \int_V \rho v_i \, dV, \tag{7}$$

and

$$\begin{aligned} \int_V \varepsilon_{ijk} x_j (b_k + b_k^E) \, dV + \int_S \varepsilon_{ijk} x_j (T_k + T_k^E) \, dS \\ = \frac{d}{dt} \int_V \rho \varepsilon_{ijk} x_j v_k \, dV. \end{aligned} \tag{8}$$

Here the components of the electrical body force b_i^E and surface traction T_i^E have been introduced. These forces arise directly from electric fields acting in the material and are in addition to the mechanical body force and surface traction. Furthermore, it is assumed that the electrical body force can be derived from the Maxwell stress tensor σ_{ij}^M such that

$$b_i^E = \frac{\partial \sigma_{ji}^M}{\partial x_j} \quad \text{in } V, \tag{9}$$

where the electrical body force is the effect of charges interacting at a distance or equivalently, the force per unit volume arising from electric fields acting on charges. The traction relationship for Maxwell stress is then

$$T_i^E = n_j \|\sigma_{ji}^M\| \quad \text{on } S. \tag{10}$$

Then, in order to satisfy the principle of conservation of linear momentum for a small surface element, the Cauchy stress in the material, σ_{ij} , must balance the total surface traction such that along with Eq. (10)

$$T_i + T_i^E = -n_j \|\sigma_{ji}\| \Rightarrow T_i = -n_j \|\sigma_{ji} + \sigma_{ji}^M\|. \tag{11}$$

The sum of the Cauchy and Maxwell stresses will be termed the total true stress, Σ_{ji} .

Next, application of Eqs. (6), (9) and (11) within the principles of conservation of linear and angular momentum and recognition that the resultant integrals must be valid for any arbitrary volume yields

$$\frac{\partial \sigma_{ji}}{\partial x_j} + \frac{\partial \sigma_{ji}^M}{\partial x_j} + b_i = \rho \frac{dv_i}{dt} \quad \text{in } V, \tag{12}$$

and

$$\sigma_{ji} + \sigma_{ji}^M = \sigma_{ij} + \sigma_{ij}^M \quad \text{in } V. \tag{13}$$

Thus, for the balance of angular momentum to be satisfied, the total true stress must be symmetric, but there is no requirement that the Maxwell and Cauchy stress tensors are individually symmetric.

3. Principle of virtual work

Now consider the rate of virtual work by agencies external to the system. This external virtual work rate, in the form relevant to the so-called electrical enthalpy, is

$$\begin{aligned} \frac{d^* \tilde{W}}{dt} = \int_V b_i v_i^* \, dV + \int_S T_i v_i^* \, dS \\ - \int_V q \frac{d^* \phi}{dt} \, dV - \int_S \omega \frac{d^* \phi}{dt} \, dS. \end{aligned} \tag{14}$$

Note that the actual work rate, involving the rate of change of charge instead of the rate of change of potential, has been given in [5], from which Eq. (14) can be found by a Legendre transformation. In Eq. (14), the asterisk indicates, respectively, a virtual differentiation with respect to time, and a virtual velocity. The material virtual rate of change of potential can be converted to spatial and convected contributions through

$$\frac{d^* \phi}{dt} = \frac{\partial^* \phi}{\partial t} - v_k^* E_k. \tag{15}$$

When this is inserted into Eq. (15), along with Eqs. (3) and (11), we obtain

$$\begin{aligned} \frac{d^* \tilde{W}}{dt} = \int_V b_i v_i^* \, dV - \int_S n_j \|\sigma_{ji} + \sigma_{ji}^M\| v_i^* \, dS \\ - \int_V q \left(\frac{\partial^* \phi}{\partial t} - v_k^* E_k \right) \, dV \\ - \int_S n_i \|D_i\| \left(\frac{\partial^* \phi}{\partial t} - v_k^* E_k \right) \, dS. \end{aligned} \tag{16}$$

Since the virtual velocity and the material virtual rate of change of potential are continuous across S , and are zero outside the domain V , the divergence theorem can now be used to convert the surface integrals to volume integrals giving

$$\begin{aligned} \frac{d^* \tilde{W}}{dt} &= \int_V \rho \frac{dv_i}{dt} v_i^* dV + \int_V (\sigma_{ji} + \sigma_{ji}^M) \frac{\partial v_i^*}{\partial x_j} dV \\ &+ \int_V D_i \frac{\partial}{\partial x_i} \left(\frac{\partial^* \phi}{\partial t} - v_k^* E_k \right) dV, \end{aligned} \quad (17)$$

where Eqs. (2) and (12) have been used to obtain a simplification. Introduction of the material virtual rate of change of the electric field then provides the PVW, namely

$$\begin{aligned} &\int_V b_i v_i^* dV + \int_S T_i v_i^* dS - \int_V q \frac{d^* \phi}{dt} dV - \int_S \omega \frac{d^* \phi}{dt} dS \\ &= \int_V \left[(\sigma_{ji} + \sigma_{ji}^M - D_j E_i) \frac{\partial v_i^*}{\partial x_j} - D_i \frac{d^* E_i}{dt} + \rho \frac{dv_i}{dt} v_i^* \right] dV \\ &= \int_V \left[(\Sigma_{ji} - D_j E_i) \frac{\partial v_i^*}{\partial x_j} - D_i \frac{d^* E_i}{dt} + \rho \frac{dv_i}{dt} v_i^* \right] dV. \end{aligned} \quad (18)$$

This form of the PVW is desirable and useful as it represents the finite strain generalization of one presented by Allik and Hughes [3] for infinitesimal strain and linearized analysis that has been available for many years. It has exactly the form needed for an up-dated Lagrangian formulation of large strain problems that is the paradigm for finite element analysis [17,18]. As such, the PVW in Eq. (18) can be the starting point for a finite element formulation for problems of electroactive materials experiencing finite strain, utilizing the physical displacements and the electric potential as the independent nodal variables. The PVW in Eq. (18) is also the one necessary for problems in which the stress-like term $D_j E_i$ is comparable in magnitude to Σ_{ji} even if the strains are infinitesimal, as can occur during switching in ferroelectrics. An additional advantage associated with the PVW in Eq. (18) is that it encompasses dissipative materials, since no constitutive information has been assumed or applied in its derivation. Furthermore, no assumption has been made regarding the nature of the Maxwell stress, the electrostrictive stress, or any other aspect of the electrostatic contributions to the state of stress. Such aspects of the problem can be assigned simply to the determination of constitutive properties of the material of interest, deduced from measurable data from such experiments, *e.g.* the dependence of the dielectric permittivity of the material on its strain [2,5]. With the formulation we have embedded in Eq. (18), we obviate the need to develop a constitutive theory that is consistent with a pre-determined formulation of the Maxwell stress, as can often be found in the literature on electroactive materials [6–16]. Instead, the constitutive model can be simplified to one that embraces simultaneously the Cauchy, Maxwell, electrostrictive and electrostatic stresses [5], which in any case cannot be separately identified from any experiment.

The PVW in Eq. (18) can be modified further by use of Eq. (5) to separate the material and aether components of the

internal virtual work, giving

$$\begin{aligned} &\int_V b_i v_i^* dV + \int_S T_i v_i^* dS - \int_V q \frac{d^* \phi}{dt} dV - \int_S \omega \frac{d^* \phi}{dt} dS \\ &= \int_V \left[(\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - P_j E_i) \frac{\partial v_i^*}{\partial x_j} - P_i \frac{d^* E_i}{dt} \right. \\ &\quad \left. + \rho \frac{dv_i}{dt} v_i^* \right] dV - \frac{d^*}{dt} \int_V \frac{1}{2} \kappa_0 E_i E_i dV \\ &= \int_V \left[(\Sigma_{ji} - \hat{\sigma}_{ji}^M - P_j E_i) \frac{\partial v_i^*}{\partial x_j} - P_i \frac{d^* E_i}{dt} \right. \\ &\quad \left. + \rho \frac{dv_i}{dt} v_i^* \right] dV - \frac{d^*}{dt} \int_V \frac{1}{2} \kappa_0 E_i E_i dV, \end{aligned} \quad (19)$$

where

$$\hat{\sigma}_{ji}^M = \kappa_0 (E_j E_i - \frac{1}{2} \delta_{ji} E_k E_k) \quad (20)$$

is the Maxwell stress in the aether. The manipulation of the aether electric field in the steps leading from Eqs. (18) to (19) can be found in [5].

4. Thermodynamics

The first law of thermodynamics states that

$$\frac{dU}{dt} = \frac{dW}{dt} + \frac{dQ}{dt}, \quad (21)$$

where U is the internal energy stored in the system, W is the external work done on the system, and Q is the heat transferred into the system. After Legendre transformation to introduce the electrical enthalpy, this becomes

$$\frac{d\tilde{U}}{dt} = \frac{d\tilde{W}}{dt} + \frac{dQ}{dt}, \quad (22)$$

where \tilde{U} is the internally stored electrical enthalpy in the system, and $d\tilde{W}/dt$ is given by the non-virtual version of Eq. (14). The rate of change of internally stored electrical enthalpy is given by

$$\begin{aligned} \frac{d\tilde{U}}{dt} &= \frac{d}{dt} \int_V \rho \tilde{u} dV - \frac{d}{dt} \int_V \frac{1}{2} \kappa_0 E_i E_i dV \\ &+ \frac{d}{dt} \int_V \frac{1}{2} \rho v_i v_i dV, \end{aligned} \quad (23)$$

where \tilde{u} is the internal electrical enthalpy stored in material per unit mass. It is convenient for later use to introduce a Helmholtz electrical enthalpy from a Legendre transformation as

$$h = \tilde{u} - \theta s, \quad (24)$$

where θ is the absolute temperature and s is the entropy of the material per unit mass. The rate of heating of the system is stated as

$$\frac{dQ}{dt} = \int_V \rho \dot{r} dV - \int_S n_i \hat{q}_i dV = \int_V \left(\rho \dot{r} - \frac{\partial \hat{q}_i}{\partial x_i} \right) dV, \quad (25)$$

where \dot{r} is the rate of heating per unit mass from internal sources (taken to be volume sources and not surface sources, so that the heat flux vector in the system is continuous), and \hat{q}_i is the heat flux vector, with the surface integral in Eq. (25) giving the heat transported out of the system through its external surface. This last statement can be made because the heat flux will be self canceling across the segments of S that represent internal divisions between regions with heterogeneous electrical properties. Such an observation calls for the appropriate treatment of the surface integral in Eq. (25), accounting for this self-cancellation. Continuity of the heat flux vector allows the divergence theorem to be used to convert the surface integral to a volume integral, as carried out for the second form of Eq. (25). The results in Eqs. (22)–(25), along with the non-virtual form of Eq. (19), allow the deduction that

$$\rho \frac{dh}{dt} = (\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - P_j E_i) \frac{\partial v_i}{\partial x_j} - P_i \frac{dE_i}{dt} - \rho s \frac{d\theta}{dt} + \rho \dot{r} - \frac{\partial \hat{q}_i}{\partial x_i} - \rho \theta \frac{ds}{dt}. \quad (26)$$

The second law of thermodynamics requires that

$$\frac{d}{dt} \int_V \rho s \, dV \geq \int_V \frac{\rho \dot{r}}{\theta} \, dV - \int_S \frac{n_i \hat{q}_i}{\theta} \, dV, \quad (27)$$

which through the divergence theorem, can be converted to

$$\rho \theta \frac{ds}{dt} \geq \rho \dot{r} - \frac{\partial \hat{q}_i}{\partial x_i} + \frac{\hat{q}_i}{\theta} \frac{\partial \theta}{\partial x_i}. \quad (28)$$

Now, combination of Eqs. (26) and (28) gives us a version of the Coleman and Noll [19] statement of the second law;

$$(\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - P_j E_i) \frac{\partial v_i}{\partial x_j} - P_i \frac{dE_i}{dt} - \rho s \frac{d\theta}{dt} - \rho \frac{dh}{dt} - \frac{\hat{q}_i}{\theta} \frac{\partial \theta}{\partial x_i} \geq 0 \quad (29)$$

which must hold for every admissible process, and gives constitutive constraints.

5. Conservative materials

The example of conservative materials will be addressed first, since it allows a prescription for identifying the constitutive law for the total true stress. These materials include non-ferroelectric piezoelectric phases of materials such as quartz and elastomers used as dielectrics in electroactive polymer actuators [20]. For a conservative material, h is a state function of the deformation, the electric field and the temperature such that

$$h = h(F_{ij}, E_i, \theta), \quad (30)$$

where $F_{ij} = \partial x_i / \partial X_j$ is the deformation gradient with X_j being the position of material points in the undeformed

configuration and x_i the position in the current configuration. As a consequence of this, Eq. (29) becomes

$$\left(\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - P_j E_i - \rho \frac{\partial h}{\partial F_{ik}} F_{jk} \right) \frac{\partial v_i}{\partial x_j} - \left(P_i + \rho \frac{\partial h}{\partial E_i} \right) \frac{dE_i}{dt} - \rho \left(s + \frac{\partial h}{\partial \theta} \right) \frac{d\theta}{dt} - \frac{\hat{q}_i}{\theta} \frac{\partial \theta}{\partial x_i} \geq 0, \quad (31)$$

which must be satisfied by all admissible processes, which are, of course, reversible. Taking each such possibility individually, we find

$$\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - P_j E_i = \rho \frac{\partial h}{\partial F_{ik}} F_{jk}, \quad (32)$$

$$P_i = -\rho \frac{\partial h}{\partial E_i}, \quad (33)$$

$$s = -\frac{\partial h}{\partial \theta}, \quad (34)$$

$$\frac{\hat{q}_i}{\theta} \frac{\partial \theta}{\partial x_i} \leq 0. \quad (35)$$

Eqs. (32)–(34) are the constitutive equations for the material, and Eq. (35) is the heat conduction condition setting a constraint on the direction of heat flux relative to the temperature gradient. Note that specification of a form for the Helmholtz function, h , determines the total true stress. As noted in previous work [5], the choice of a formula for the Maxwell stress is not freely disposable, but must instead be made in a manner consistent with the constitutive law chosen to characterize the material behavior. The resulting form is equivalent to a combination of what are often separately denoted the Maxwell and electrostrictive stresses [2,10,13]. In any case, it is impossible to separately measure the Cauchy, Maxwell and electrostrictive stresses [2,5,10,13], so the distinction is immaterial. It is only necessary to focus on the total true stress, Σ_{ji} .

Objectivity requires that the Helmholtz function depends on rotation invariant measures [21]. These rotation invariant measures must encompass both the deformation and the electrical terms appearing as arguments of h . To implement this, we set $h = h(\varepsilon_{ij}, e_i, \theta)$, where the Green–Lagrange strain, ε_{ij} , is given by [21]

$$\varepsilon_{ij} = \frac{1}{2}(F_{ki} F_{kj} - \delta_{ij}), \quad (36)$$

and the rotation invariant electric field, e_i , is

$$e_i = E_j R_{ji}, \quad (37)$$

in which R_{ji} is the orthogonal tensor obtained upon polar decomposition of the displacement gradient [21]. Note that instead of e_i we could have chosen to use the electric field defined in material coordinates, $-\partial \phi / \partial X_i = E_j F_{ji}$ to ensure objectivity of h . However, to retain formulations most suitable to an up-dated Lagrangian approach, and also due to previous work [5], it is more convenient to employ e_i , and to use derivation already provided in our previous paper. With objectivity

ensured, Eqs. (32) and (33) are replaced by

$$\begin{aligned}\Sigma_{ji} &= \sigma_{ji} + \sigma_{ji}^M \\ &= \rho \frac{\partial h}{\partial \varepsilon_{lm}} F_{jm} F_{il} + \beta_{jikl} P_k E_l + P_j E_i + \hat{\sigma}_{ji}^M,\end{aligned}\quad (38)$$

and

$$P_i = -\rho R_{ij} \frac{\partial h}{\partial e_j}, \quad (39)$$

in which β_{jikl} is given by [5,22]

$$\begin{aligned}\beta_{jikl} &= \frac{1}{v} V_{jm} (V_{nn} \delta_{mp} - V_{mp}) (V_{qq} \delta_{ir} - V_{ir}) \\ &\quad \times (\delta_{rk} \delta_{pl} - \delta_{rl} \delta_{pk}),\end{aligned}\quad (40a)$$

$$v = \text{Det}(V_{kk} \delta_{ij} - V_{ij}) = \text{Det}(U_{kk} \delta_{ij} - U_{ij}), \quad (40b)$$

in which U_{ij} and V_{ij} are the right and left Cauchy–Green tensors from the polar decomposition of the displacement gradient as in [21]

$$F_{ij} = R_{ik} U_{kj} = V_{ik} R_{kj}. \quad (41)$$

As noted in [5], the form of β_{jikl} is such that $\Sigma_{ji} = \sigma_{ji} + \sigma_{ji}^M$ as given by Eq. (38) is symmetric, thereby ensuring conservation of angular momentum.

The result in Eq. (38) makes it clear that the Maxwell stress must have a form consistent with the Helmholtz function that defines the conservative behavior of the material [5]. Examples of the consequences of this restriction are given in [5], where it is emphasized that assumptions about the form of the Maxwell, electrostrictive and electrostatic stresses cannot be made independently of the constitutive law governing the material behavior.

6. Dissipative materials

This class of systems includes switchable ferroelectrics [1] and viscoelastic materials used as the dielectric of electroactive polymer actuators [20]. To formulate the equations for these systems, we use the standard concept where dissipative processes are taken to be a sequence of constrained equilibrium configurations [23–25]. That is, to interpret Eq. (29), we consider the state of the material at each stage to be fixed in that internal variables involved in the dissipative processes are held stationary, and equilibrium thermodynamics is used to analyze each configuration.

Following Coleman and Gurtin [24], we consider the Helmholtz electrical enthalpy to be dependent on a set of internal variables, ξ_i , that control the dissipative material processes in addition to its dependence on strain, electric field and temperature. Thus,

$$h = h(\varepsilon_{ij}, e_k, \theta, \xi_l). \quad (42)$$

Use of Eq. (42) in Eq. (29) provides

$$\begin{aligned}&\left(\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - \beta_{jikl} P_k E_l - P_j E_i - \rho \frac{\partial h}{\partial \varepsilon_{kl}} F_{jk} F_{il} \right) \frac{\partial v_i}{\partial x_j} \\ &\quad - \left(P_i + \rho R_{ik} \frac{\partial h}{\partial e_k} \right) \frac{dE_i}{dt} - \rho \left(s + \frac{\partial h}{\partial \theta} \right) \frac{d\theta}{dt} \\ &\quad + \rho f_i \frac{d\xi_i}{dt} - \frac{\hat{q}_i}{\theta} \frac{\partial \theta}{\partial x_i} \geq 0,\end{aligned}\quad (43)$$

where

$$f_i = -\frac{\partial h(\varepsilon_{jk}, e_l, \theta, \xi_m)}{\partial \xi_i} \quad (44)$$

are the conjugate thermodynamic forces acting on the internal variables. The number of internal variables included in the summation in Eq. (43) is that present in a unit mass of the material. As with Eq. (32), this inequality must prevail for all possible admissible processes. The same arguments lead to the equivalents of Eqs. (32), (33), (38) and (39), rephrased as

$$S_{ij} = \rho_0 \frac{\partial h(\varepsilon_{kl}, e_m, \theta, \xi_n)}{\partial \varepsilon_{ij}}, \quad (45)$$

$$\Pi_k = -\rho_0 \frac{\partial h(\varepsilon_{ij}, e_l, \theta, \xi_m)}{\partial e_k}, \quad (46)$$

where

$$S_{mn} = \frac{\rho_0}{\rho} F_{mi}^{-1} F_{nj}^{-1} (\sigma_{ji} + \sigma_{ji}^M - \hat{\sigma}_{ji}^M - \beta_{jikl} P_k E_l - P_j E_i) \quad (47)$$

is an electromechanical 2nd Piola–Kirchhoff stress [21],

$$\Pi_k = \frac{\rho_0}{\rho} P_i R_{ik} \quad (48)$$

is a rotation invariant polarization [5] relative to unit reference volume, so that it represents the dipole moment per unit reference volume, and ρ_0 is the density of material in the reference state. Eqs. (45) and (46) represent the reversible response of the material behavior in its constrained equilibrium state since the internal variables, ξ_j , are held fixed. These results are actually identical in form to the expressions given in Eqs. (38) and (39), although expressed in terms of different variables. This makes it clear that the form of the Maxwell stress, embedded in S_{ij} , must be consistent with the form of the Helmholtz function governing the conservative constitutive response of the material. This situation is completely analogous to the deductions drawn from Eqs. (38) and (39) in the case of the purely conservative materials, with examples of the consequences presented previously in [5]. Thus, if the conservative part of the constitutive law of the dissipative material is identical to the constitutive law of a purely conservative material, then the form of the Maxwell stress in the dissipative material is the same as that in the purely conservative material. As noted previously, examples of the consequences of constitutive assumptions for the form of the Maxwell, or electrostatic, stress have been given in [5]. Note that Eq. (34) still provides the entropy, and the heat

conduction inequality is still given by Eq. (35). Finally, the remaining condition from Eq. (43),

$$f_i \frac{d\zeta_i}{dt} \geq 0, \quad (49)$$

previously noted by Coleman and Gurtin [24] and Rice [25], confirms that the reconfiguration of internal variables is indeed a dissipative process.

7. Constitutive law structure for dissipative materials

To complete the construction of a form of a constitutive law for a dissipative material, we follow Rice [25] by introducing a Legendre transformation to provide the Gibbs free energy function defined by

$$g(S_{kl}, e_m, \theta, \zeta_n) = \varepsilon_{ij} \frac{\partial h}{\partial \varepsilon_{ij}} - h. \quad (50)$$

The difference in the Gibbs free energy function between two neighboring constrained states is

$$\delta g = \frac{1}{\rho_0} \varepsilon_{ij} \delta S_{ij} + \frac{1}{\rho_0} \Pi_k \delta e_k + f_l \delta \zeta_l + s \delta \theta, \quad (51)$$

where δ indicates the difference in the parameter following it between the two neighboring constrained states. Eq. (51) leads to

$$\varepsilon_{ij} = \rho_0 \frac{\partial g(S_{kl}, e_m, \theta, \zeta_n)}{\partial S_{ij}}, \quad (52)$$

$$\Pi_k = \rho_0 \frac{\partial g(S_{ij}, e_l, \theta, \zeta_m)}{\partial e_k}, \quad (53)$$

$$f_i = \frac{\partial g(S_{jk}, e_l, \theta, \zeta_m)}{\partial \zeta_i}, \quad (54)$$

$$s = \frac{\partial g(S_{ij}, e_k, \theta, \zeta_l)}{\partial \theta}. \quad (55)$$

Maxwell relationships derived from these equations provide

$$\frac{\partial \varepsilon_{ij}}{\partial \zeta_k} = \rho_0 \frac{\partial f_k}{\partial S_{ij}}, \quad (56)$$

$$\frac{\partial \Pi_i}{\partial \zeta_k} = \rho_0 \frac{\partial f_k}{\partial e_i}. \quad (57)$$

The increment of irreversible strain between neighboring constrained states (remanent strain plus an increment of strain response caused by changes in the conservative properties of the material associated with the reconfiguration of the internal variables) is generated by the difference in internal variables between them, so that

$$\begin{aligned} \delta \varepsilon_{ij}^{\text{irr}} &= \frac{\partial \varepsilon_{ij}(S_{lm}, e_n, \theta, \zeta_p)}{\partial \zeta_k} \delta \zeta_k \\ &= \rho_0 \frac{\partial f_k(S_{lm}, e_n, \theta, \zeta_p)}{\partial S_{ij}} \delta \zeta_k. \end{aligned} \quad (58)$$

The increment of irreversible polarization between neighboring constrained states (remanent polarization plus an increment of

polarization response caused by changes in the conservative properties of the material associated with the reconfiguration of the internal variables) is generated by

$$\begin{aligned} \delta \Pi_i^{\text{irr}} &= \frac{\partial \Pi_i(S_{jl}, e_m, \theta, \zeta_n)}{\partial \zeta_k} \delta \zeta_k \\ &= \rho_0 \frac{\partial f_k(S_{jl}, e_m, \theta, \zeta_n)}{\partial e_i} \delta \zeta_k. \end{aligned} \quad (59)$$

In the above two equations, it is necessary to recognize the increments of strain and polarization that are possibly embedded in Eqs. (58) and (59) due to the fact that ferroelectrics experience a change in their dielectric, elastic and piezoelectric properties during ferroelectric switching by domain wall motion, leading to a reconfiguration of the internal domain structure of the material. For example, an unpoled ferroelectric material is initially isotropic, and thus not piezoelectric, whereas poling induces piezoelectric response, so that as the internal variables change (*i.e.* the domain volume fractions and the location of the domain walls change), the reversible, conservative portion of the strain and polarization will vary even as the stress and electric field are held fixed [1]. Thus the portions of the strain and polarization increments that we call irreversible are, in general, the remanent amounts plus contributions that are generated by the changing properties of the material that occur as the internal variables are reconfigured.

Following Rice [25] again, assume that the rate of change of the internal variables depends only on the thermodynamic forces applied to them, the temperature and the internal variables themselves so that

$$\frac{d\zeta_i}{dt} = \dot{\zeta}_i = \dot{\zeta}_i(f_j, \theta, \zeta_k). \quad (60)$$

Then introduce a rate potential scalar function Ω , defined by

$$\Omega(S_{ij}, e_k, \theta, \zeta_l) = \rho_0 \int_0^{\dot{\zeta}_i(\varepsilon_{ij}, e_k, \theta, \zeta_l)} \dot{\zeta}_i(f_j, \theta, \zeta_k) d f_i. \quad (61)$$

From this there follows

$$\begin{aligned} \frac{\partial \Omega(S_{ij}, e_k, \theta, \zeta_l)}{\partial S_{mn}} &= \rho_0 \dot{\zeta}_p(f_q, \theta, \zeta_r) \frac{\partial f_p(S_{qr}, e_s, \theta, \zeta_t)}{\partial S_{mn}} \\ &= \dot{\varepsilon}_{mn}^{\text{irr}} \end{aligned} \quad (62)$$

and

$$\begin{aligned} \frac{\partial \Omega(S_{ij}, e_k, \theta, \zeta_l)}{\partial e_m} &= \rho_0 \dot{\zeta}_p(f_q, \theta, \zeta_r) \frac{\partial f_p(S_{qr}, e_s, \theta, \zeta_t)}{\partial e_m} \\ &= \dot{\Pi}_m^{\text{irr}}, \end{aligned} \quad (63)$$

where Eqs. (58), (59) and (61) have been used in these results. Eqs. (62) and (63) confirm that Ω is indeed a rate potential, generating both the irreversible part of the strain rate and the irreversible part of the polarization rate of change.

The complete constitutive law can be constructed by combining the reversible, conservative response with the rate of change of the irreversible strain and polarization, such that

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{\text{rev}} + \dot{\varepsilon}_{ij}^{\text{irr}}, \quad (64)$$

and

$$\dot{\Pi}_i = \dot{\Pi}_i^{\text{rev}} + \dot{\Pi}_i^{\text{irr}}, \quad (65)$$

where the superscript rev indicates the conservative, reversible portion of the relevant rate, and the superposed dot indicates the time rate of change. Eqs. (52) and (53) are used to provide the reversible conservative response and the complete constitutive law is then given by

$$\dot{\epsilon}_{ij} = \rho_0 \frac{\partial^2 g}{\partial S_{ij} \partial S_{kl}} \dot{S}_{kl} + \rho_0 \frac{\partial^2 g}{\partial S_{ij} \partial e_k} \dot{e}_k + \rho_0 \frac{\partial^2 g}{\partial S_{ij} \partial \theta} \dot{\theta} + \frac{\partial \Omega}{\partial S_{ij}}, \quad (66)$$

$$\dot{\Pi}_i = \rho_0 \frac{\partial^2 g}{\partial e_i \partial S_{kl}} \dot{S}_{kl} + \rho_0 \frac{\partial^2 g}{\partial e_i \partial e_k} \dot{e}_k + \rho_0 \frac{\partial^2 g}{\partial e_i \partial \theta} \dot{\theta} + \frac{\partial \Omega}{\partial e_i}. \quad (67)$$

These results are analogous to Rice's [25] Eq. (21), which addressed plasticity. We have thus extended his analysis to include electromechanically responsive materials such as switchable ferroelectrics and viscoelastic-electrostrictive materials. It should be noted that Rice [25] extended his result to encompass the case of rate independent materials having a yield surface rather than a rate potential to generate the inelastic component of the strain rate. We could do so also to extend Eqs. (66) and (67) to a rate independent special case, but we will take that as given already by Rice [25]. Nevertheless, we note that Landis [26] and McMeeking and Landis [27] have developed rate independent constitutive laws that conform to the framework of Eqs. (66) and (67). Landis' [25] and McMeeking's and Landis' [27] laws omit the Maxwell stress, ignore temperature change, and are specialized to infinitesimal strain. However, we now see that their constitutive formulations are consistent with the notions of internal variables controlling the internal dissipative reconfiguration of the material and the associated thermodynamic theory. It follows that these constitutive laws can be made valid for arbitrary conditions by adding the electrostatic stress contributions that are consistent with the assumed form of the Helmholtz free energy used in their treatments.

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