On the use of thermodynamic formalism in generalized continuum theories and a model for damage evolution

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Abstract

A technique for setting up generalized continuum theories based on a balance law and nonlocal thermodynamics is suggested. The methodology does not require the introduction of gradients of the internal variable in the free energy while allowing for its possibility. Elements of a generalized (brittle) damage model with porosity as the internal variable are developed as an example. The notion of a flux of porosity arises, and we distinguish between the physical notion of a flux of voids (with underpinnings of corpuscular transport) and a flux of void volume that can arise merely due to void expansion. A hypothetical, local free energy function with classical limits for the damaged stress and modulus is constructed to show that the model admits a nonlinear diffusion-advection equation with positive diffusivity for the porosity as a governing equation. This equation is shown to be intimately related to Burgers equation of fluid dynamics, and an analytical solution of the corresponding constant-coefficient, semilinear equation without source term is solved by the Hopf-Cole transformation, that admits the Hopf-Lax entropy weak solution for the associated Hamilton-Jacobi equation in the limit of vanishing diffusion. Constraints on the class of admissible porosity and strain-dependent free energy functions arising from the mathematical structure of the theory are deduced. This work may be thought of as providing a continuum thermodynamic formalism for the internal variable gradient models proposed by Aifantis (1984) in the context of *local* stress and free-energy functions. However, the degree of diffusive smoothing is not found to be arbitrarily specifiable as mechanical coupling produces an 'anti-diffusion' effect, and the model also inextricably links propagation of regions of high gradients with their diffusive smoothing.

1. Introduction

In formulating generalized continuum theories with a gradient of an internal variable, use is often made of a postulated principle of virtual power (or an equivalently postulated microforce balance) and/or an inclusion of the gradient term in the free-energy with subsequent utilization of the Second Law. Depending upon taste, such postulation may or may not seem to be sufficiently physically motivated, at least in terms of operational definitions of the various microforces involved and their experimental observation/measurement. Less subjectively, the above techniques rely crucially on the explicit dependence of the free energy on the gradient term, and such an additional contribution to the free energy can be shown to be superfluous at least in one context, suggesting that some caution should be exercised in following this approach. In this article, I demonstrate the above superfluity through an explicit example related to dislocation mechanics.

As an alternative strategy to formulating generalized theories, I suggest the choice of a physically clear kinematic variable (that could be a gradient of an internal variable) along with the discovery, or use of an already-existing, equally clear evolution statement in the form of a balance law that is essentially kinematical before the introduction of constitutive statements for the flux and source terms. Second, a free energy function with a 'correct' dependence on the state variables, which may very well not include a dependence on the added kinematic (gradient) variable, is considered important. With these ingredients in hand and use of the Coleman-Noll-

Gurtin Second Law apparatus, at least in spirit if not in details, a closed theory, up to details of constitutive dependencies on derived driving forces, can be developed.

These ideas are demonstrated in the context of a generalized continuum theory for void volume fraction evolution in an otherwise elastic material. Interestingly, the model suggests that one may have a diffusive effect in damage evolution only if the strain energy function depends upon the void volume fraction more than linearly, thus raising the physical question of the appropriate dependence of the homogenized elastic modulus on void volume fraction at high void volume fraction. The development of nonlocal models of damage is an extensive field with many models as described in the excellent review section in Peerlings et al. (2004), beginning with the pioneering works of Bazant (1984) and Bazant and Pijaudier-Cabot (1988); in most cases, the introduction of the nonlocal terms in the constitutive structure do not translate to directly identifiable physical mechanisms that can then be a guide for experimental characterization or computation from homogenization. The addition to this huge literature with yet another model in this article may perhaps be excused due to its intended emphasis on physical transparency: the damage variable is the void volume fraction, a well identifiable quantity. Being a density, the evolution of this damage variable, *of necessity*, has to fit into the structure of a balance law. A material control volume has its content of void volume altered by voids/cracks entering into it through its bounding surface that may be interpreted as a flux of *void volume*; the extension of cracks and voids necessarily involve dissipation as at the atomistic level these are very dynamic events and thus the flux of void volume may be interpreted as dissipative in origin. And, finally, the free energy of a solid must necessarily depend upon the void volume content, as in the limit when the void volume fraction is unity there is no solid left and hence no corresponding stored energy, while for the unvoided material the solid has stored energy when strained due to deformation of atomic bonds – more convincingly, homogenization results for a solid containing a dilute concentration of voids always show at least a dependence of the elastic moduli on the void volume fraction (e.g. Nemat-Nasser and Horii, 1999).

As for connections with prior work, the final outcome of the methodology suggested here is a special case of Gurtin's generalized Cahn-Hilliard equations (1996), but without the use of a microforce balance. These latter equations are fourth-order diffusive PDE in the order parameter with a singular perturbation structure, related to the introduction of the gradient of the order parameter into the free energy function to provide stabilization to the ill-posed, backward heat equation that arises near a spinodal decomposition in phase transforming continua, as described in Cahn (1961). In contrast, the central hypothesis in this work relates to not necessarily including a gradient term in the free energy, and the second-order spatial differential operator that arises in our equations appears in a physically natural manner to be a stabilizing, diffusive effect.

There are also stabilizing, second-order PDEs in the internal variable/order parameter field that arise in the framework of Ginzburg-Landau/Allen-Cahn equations in materials science. Gurtin's (1996) work contains a generalization of these equations for coupling with deformation, in the framework of a microforce balance. Menzel and Steinmann's (2000) work may be considered as an application to plasticity of such equations. Of course, the appearance of the stabilizing second-order spatial differential operator in these works hinges crucially on the presence of the gradient of the order parameter field in the free energy, and it is in this respect that the present work differs from the above.

In summary, the general class of models presented here takes on an intermediate position between deformation-coupled Ginzburg-Landau/Allen-Cahn equations and the Cahn-Hilliard

equations. The framework produces second-order PDE in the order parameter/internal variable field without the presence of a gradient in the free energy function but due to the fact that the order parameter satisfies a balance law.

A balance law for a field variable, before the introduction of constitutive quantities, is a tautological statement that arises from merely the physical definition of the variable. As such, it is to be satisfied as a *necessary condition* by that field regardless of whether its evolution is defined by the balance law itself or some other constitutive statement, and this fact poses restrictions on constitutive equations. While such an unequivocal statement cannot in general be made about a generic type of dependence of the specific free energy on the internal variable/order parameter, well-founded choices generalizing experience and homogenization theory for micromechanics can be made, and these two ingredients seem to suggest a pathway to defining reasonable models of inhomogeneous continuum response.

2. Explicit dependence of specific free energy on internal variable is not always correct: elastic dislocation theory as an example

The order parameter/internal variable in the elastic theory of dislocations is the Nye (1953) dislocation density tensor. However, it is a well-known standard result (see, e.g., Kröner, 1981, Sec. 4) that the strain energy density of a dislocation distribution (including individual discrete dislocations) depends only on the elastic strain that results from the dislocation density distribution and not on *both* the elastic strain and the dislocation density. Furthermore, this strain energy density function corresponds to the linear elastic stress and strain fields of the dislocation distribution involved, as the latter fields are understood in classical dislocation theory (e.g., Nabarro, 1987). In what follows in this section, this result is illustrated in the context of standard procedures for solving boundary value problems in continuum inelasticity theory, one goal being to demonstrate that such calculations may be performed without recourse to Green's functions and infinite media and through equations ideally suited for numerical computation with the finite element method.

Consider the following question: we are interested in determining the state of internal stress and the strain energy in a linear elastic body of given geometry, for a prescribed dislocation density field $\boldsymbol{\alpha}$. For definiteness, the prescribed dislocation density field can be thought of as representing a screw dislocation along a straight cylinder representing its core. While the main conclusion of this section applies at all instants of time in the deformation of a body, it suffices to demonstrate the idea at any one instant and we choose the initial instant for definiteness. Thus, the problem may be thought of as determining the initial condition on the plastic distortion field in a conventional elastoplasticity calculation, where the plastic distortion field, $\boldsymbol{U}^p$, has to satisfy

$$curl\, \boldsymbol{U}^p = -\boldsymbol{\alpha}\,. \tag{1}$$

Thus, we need to solve the equations

$$\begin{aligned} &div\left[\boldsymbol{C}\boldsymbol{U}^e\right] = \boldsymbol{0} \\ &\boldsymbol{U}^e + \boldsymbol{U}^p = grad\, \boldsymbol{u} \\ &curl\, \boldsymbol{U}^e = -curl\, \boldsymbol{U}^p = \boldsymbol{\alpha}, \end{aligned} \tag{2}$$

and since we are talking about initial conditions (for an elastoplasticity calculation), the displacement $\boldsymbol{u} \equiv \boldsymbol{0}$ at the initial time so that $\boldsymbol{U}^e = -\boldsymbol{U}^p$ at this time. Here, $\boldsymbol{C}$ is the possibly anisotropic linear elastic moduli with major and minor symmetries and $\boldsymbol{U}^e$ is the elastic

distortion. In classical elastoplasticity, (2) is appended with an evolution equation for $\boldsymbol{U}^p$ or its symmetric part. For this problem (2) at the initial time when the displacement is known, we consider statically consistent traction boundary conditions (possibly vanishing) to be specified. The paper of Willis (1967) shows that solving these equations amounts to solving the problem of internal stress in classical dislocation theory corresponding to the prescribed dislocation density field. The existence of a non-trivial initial dislocation density distribution in the body is an eminently physical statement; the associated possibility of a non-trivial, *initial* plastic distortion in any theory where the fundamental relation (1) is active reflects the physical fact that the instantaneous dislocation density distribution encodes information of some portion of the past history of dislocation motion/nucleation in the body.

To solve the problem in the format of continuum inelasticity, we first note that it can be shown that there is at most one solution to the problem of calculating the initial distribution of stress, $\boldsymbol{T} = \boldsymbol{C}\boldsymbol{\varepsilon}^e$, where $\boldsymbol{\varepsilon}^e$ is the symmetric part of $\boldsymbol{U}^e$. Thus, as long as we can solve (2) and the associated boundary conditions by any procedure, the resulting solution would be the correct one. To find this solution, represent the plastic distortion as a sum of a gradient of a vector field and a tensor field whose *curl* does not vanish as

$$\boldsymbol{U}^p \coloneqq -\boldsymbol{\chi} + grad\, \boldsymbol{z} \tag{3}$$

so that

$$-curl\, \boldsymbol{U}^p = \boldsymbol{\alpha} \Rightarrow curl\, \boldsymbol{\chi} = \boldsymbol{\alpha}\,. \tag{4}$$

In order to solve for $\boldsymbol{\chi}$ in a well-posed manner, we append the equations

$$\begin{aligned} &div\, \boldsymbol{\chi} = \boldsymbol{0} \\ &\boldsymbol{\chi}\boldsymbol{n} = \boldsymbol{0} \ \text{ on boundary} \end{aligned} \tag{5}$$

to (4) to obtain a Poisson's equation

$$div\, grad\, \boldsymbol{\chi} = -curl\, \boldsymbol{\alpha} \tag{6}$$

for the components of the tensor $\boldsymbol{\chi}$ with Dirichlet boundary conditions; this problem may be solved by standard methods of potential theory.

With a solution for $\boldsymbol{\chi}$ in hand, one solves the equilibrium equation

$$div\big[-\boldsymbol{C}\, grad\, \boldsymbol{z}\big] = div\big[\boldsymbol{C}\boldsymbol{\chi}\big] \tag{7}$$

for the vector field $\boldsymbol{z}$ with Neumann boundary conditions inferred from the prescribed traction boundary condition and the boundary values of the field $\boldsymbol{\chi}$. This is a standard problem in linear elasticity theory. The solution for $grad\, \boldsymbol{z}$ is unique, and this is all that matters for the present purpose.

The fields $grad\, \boldsymbol{z}$ and $\boldsymbol{\chi}$ in conjunction with (3) and $\boldsymbol{u} \equiv \boldsymbol{0}$ now deliver the solution to (2) and thus the unique elastic strain and stress fields corresponding to the prescribed dislocation density field $\boldsymbol{\alpha}$, including arbitrary discrete dislocations in finite, anisotropic, linear elastic bodies.

The corresponding elastic strain energy density distribution in the body, consistent with the classical elastic theory of dislocations, is given by

$$\bar{\psi}\left(\boldsymbol{\varepsilon}^e\right) \coloneqq \frac{1}{2}\left(\boldsymbol{C}\,\boldsymbol{\varepsilon}^e\right) : \boldsymbol{\varepsilon}^e \quad ; \quad \boldsymbol{\varepsilon}^e \coloneqq \left(-grad\, \boldsymbol{z} + \boldsymbol{\chi}\right)_{sym} = \boldsymbol{U}^e_{sym} \tag{8}$$

and, consequently, an assumption of the form

$$\psi = \bar{\psi}\left(\boldsymbol{\varepsilon}^e\right) + \hat{\psi}\left(\boldsymbol{\alpha}\right) \tag{9}$$

would be superfluous and physically inaccurate in this context where core effects are not taken into account.

3. Elements of a nonlocal damage model based on thermodynamics and a necessary balance law of kinematical origin

It has been well-understood for some time now that classical local theories of continuum mechanics are inadequate for dealing with stress-softening response and the prediction of associated length scale effects. Both these physical features are an essential ingredient of materials that have been damaged due to the production of microcavities in them. Bazant (1984) was the first to realize that a proper theoretical treatment of such effects would require consideration of some sort of non-local effects in material response. Thus, an integral/gradient measure of some effective strain or a 'damage' variable has been introduced in the elastic stiffness, strain energy, or the strength of the material (cf. Pijaudier Cabot and Bazant, 1988; Aifantis, 1984; Peerlings at al. 2004; Lorentz and Andrieux, 1999; Liebe et al. 2001). When the damage variable is identified with some representation of voids so that a spatial region with a high gradient in this variable may be grossly interpreted as a boundary between very differently voided region and, in the limit, as a microcavity surface, the inclusion of such gradient in the free energy may be justified as a continuum accounting of surface energy. Except for this case, it is perhaps fair to say that the other devices used for introducing a nonlocal effect in damage are left somewhat wanting in terms of physical justification of the means adopted to do so.

In contrast, the model presented here is based on the four assumptions that follow:

1. The physical body containing voids is thought of as a set of points, as is usual in continuum mechanics. Each point is endowed with a void volume fraction attribute, defined physically as the limit of the ratio of the volume of voids in a region to the volume of the region, as the volume of the region goes to zero. The void volume fraction field on the body naturally varies with time. This field is identified as the damage variable of the model, physically representative of a density of microcavity volume in the material. We denote it with the symbol $\varphi \in [0,1]$.
2. The linear elastic moduli, and therefore the specific free energy, of the voided material depends on the void volume fraction. This is physically intuitive as well as supported by micromechanics studies (e.g. Nemat-Nasser and Horii, 1999). Thus, the specific free energy of the material depends, as a first approximation, only on elastic strain and the void volume fraction. In particular, *the specific free energy of the material does not depend on a gradient of the damage variable*.
3. The void volume fraction, defined as above, is a volumetric density. Therefore, its evolution, *regardless of how it is specified, constitutively or otherwise,* can *necessarily* be expressed as a balance law. For, if we focus on any arbitrarily fixed region in the body, it is a purely kinematic argument that the rate of change of the void volume contained in that region changes due to the production of new voids and due to the influx of void volume content from the ingress of microcracks/cavities into that volume from its exterior. *It should be carefully noted that a flux of void volume through a surface is not necessarily to be identified with a transport of entire voids through the surface, each void considered as an entity. Instead the expansion/contraction of the voids causes the flux in void volume that is relevant for this discussion. In other words, void transport is sufficient for transport of void volume, but not necessary*. Thus, the

flux of void volume may be linked to the transport of infinitesimal elements of void-solid interface instead of entire voids. We make the usual assumption of continuum mechanics that given an oriented plane surface with normal $\boldsymbol{n}$ through a point $\boldsymbol{x}$ there exists a flux vector $\boldsymbol{f}$ as a function of $\boldsymbol{x}$ such that $\boldsymbol{f}\cdot\boldsymbol{n}$ equals the flux of void volume per unit area per unit time through the plane area at $\boldsymbol{x}$ in the direction $-\boldsymbol{n}$. Thus, in the situation when the point $\boldsymbol{x}$ resides on the surface of a closed volume and $\boldsymbol{n}$ is the outward unit normal at $\boldsymbol{x}$ with respect to the closed volume, $\boldsymbol{f}\cdot\boldsymbol{n}$ characterizes the inward flow of void volume per unit area per unit time *into* the body at $\boldsymbol{x}$.

4. We assume that the dissipated mechanical energy characterized by the rate of working of the external loads less the rate of change of free energy and kinetic energy of the body is always non-negative in any physical process of the body:

$$D = \int_{\partial B} \boldsymbol{t}\cdot\dot{\boldsymbol{u}}\, da + \int_B \boldsymbol{b}\cdot\dot{\boldsymbol{u}}\, dv - \frac{d}{dt}\int_B \left(\psi + \rho|\dot{\boldsymbol{u}}|^2\right) dv \geq 0 \tag{10}$$

Here, $\boldsymbol{t}$ is the applied traction on the external surface of the body, $\boldsymbol{u}$ is the displacement field, $\boldsymbol{b}$ is the body force density, ψ is the free energy density field and ρ is the mass density.

Using standard arguments of continuum mechanics involving localizing integral statements of balance, Assumption 3 above implies that the void volume fraction field satisfies

$$\dot{\varphi} = div\, \boldsymbol{f} + s \tag{11}$$

where s is a nucleation rate of void volume fraction. Assumption 2 above implies a free energy function of the form

$$\psi = \psi(\boldsymbol{\varepsilon}, \varphi), \tag{12}$$

where $\boldsymbol{\varepsilon}$ is the strain tensor given by the symmetric part of the displacement gradient. Assumption 4 along with balance of linear momentum implies that

$$D = \int_B \boldsymbol{T} : \dot{\boldsymbol{\varepsilon}}\, dv - \int_B \dot{\psi}\, dv \geq 0, \tag{13}$$

where $\boldsymbol{T}$ is the stress tensor, and assuming elastic behavior in the absence of void evolution, i.e.

$$\boldsymbol{T} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \tag{14}$$

we have

$$D = \int_B -\frac{\partial \psi}{\partial \varphi}\, \dot{\varphi}\, dv \geq 0. \tag{15}$$

For simplicity we assume that no voids are introduced into the body through its external boundaries. Then, substituting (11) in (15) exposes the driving forces for the flux and the source terms as the multipliers of the terms $\boldsymbol{f}$ and s in

$$D = \int_B \left[-grad\, Y\cdot\boldsymbol{f} + Ys\right] dv, \quad Y := -\frac{\partial \psi}{\partial \varphi}, \tag{16}$$

in the sense that in the absence of these driving forces absence the physical mechanisms of the void volume fraction flux and nucleation could occur without any dissipation of energy, a clearly unphysical statement as at the atomic level, crack/microcavity propagation or nucleation are dynamic events that result in energy transfer into incoherent atomic vibrations that cannot be represented at coarser time and length scales by the continuum displacement field.

The driving force Y for void volume fraction nucleation is standard from the thermodynamics of local damage models. It is instructive to write the driving force for the flux in the form

$$-grad\, Y = \frac{\partial^2 \psi}{\partial \varphi^2} grad\, \varphi + \frac{\partial^2 \psi}{\partial \varphi \partial \boldsymbol{\varepsilon}} : grad\, \boldsymbol{\varepsilon} \tag{17}$$

and note that this model implies that there cannot be a thermodynamic force for void flux unless the free energy depends upon the void volume fraction more than linearly. Assuming the simplest possible linear, isotropic constitutive response for the flux of the form

$$\boldsymbol{f} = B\left(-grad\, Y\right), \quad B \geq 0\,, \tag{18}$$

where B is a material parameter required on dimensional grounds, we obtain a 'diffusive' evolution equation of the form

$$\dot{\varphi} = div\left(B \frac{\partial^2 \psi}{\partial \varphi^2} grad \varphi \right) + div\left(B \frac{\partial^2 \psi}{\partial \varphi \partial \boldsymbol{\varepsilon}} : grad\, \boldsymbol{\varepsilon} \right) + s\,, \tag{19}$$

with s characterized by a local constitutive equation ensuring $Ys \geq 0$. For stable response it is necessary that

$$\partial^2 \psi / \partial \varphi^2 > 0\,, \tag{20}$$

implying a decrease in driving force for cavity nucleation with increase in porosity.

It is also important to note that a physical length-scale enters the problem through the material parameter B. Of course, as stated the model would be rate dependent due to the time-dependence of the diffusion term, but it is a straightforward matter to make appropriate modifications for empirically postulated rate-independent response as well as more complicated constitutive rules. Due to the clear meaning of the diffusive flux term, it may be expected that the constant B could be determined from experiments measuring work done in damage evolution. It is clear from (19) that this generalized model of damage provides a diffusive stabilization opposing a localization of damage on to a surface of discontinuity. Apart from this diffusive effect, the model implies that the evolution of void volume fraction is dependent on the Laplacian as well as the first gradient of the strain tensor field, spatially 'nonlocal' effects that are absent in local damage models.

It is interesting to expand (19) in the form

$$\dot{\varphi} = B \partial_{\varphi\varphi} \psi \underbrace{div\, grad\, \varphi}_{Laplacian\, \varphi} + \left(B \partial_{\varphi\varphi\varphi} \psi \right) grad\, \varphi \cdot grad\, \varphi + \cdots \tag{21}$$

and note that, for $\partial_{\varphi\varphi\varphi} \psi \neq 0$, the model admits traveling wave solutions for the void volume fraction (at least in the linearized setting), reflecting the motion of smoothed interfaces between void and solid.

4. A 1-d Example

In this section we derive the governing equation for the extension of an elastic bar with damage. Since the backward heat equation (i.e. with negative coefficient of the Laplacian) can be entirely unstable, a primary goal is to see whether a free energy function that yields classical expressions for the stress and the elastic modulus is at least mathematically possible for which one obtains a forward diffusion operator in the porosity evolution in the governing equations of the model.

Consider a 1-d elastic bar under tension capable of developing damage through the development of a porosity distribution. The axis of the bar is aligned with the x coordinate direction. Let the free energy function be $\psi(\varepsilon, \varphi)$ where $\varepsilon = \partial u / \partial x$, and u is the axial displacement. Static equilibrium requires

$$\frac{\partial}{\partial x}\left[\frac{\partial \psi}{\partial \varepsilon}(\varepsilon,\varphi)\right]=0, \tag{22}$$

where the axial stress is $\partial\psi/\partial\varepsilon$. Thus, (22) implies

$$\frac{\partial \varepsilon}{\partial x}=-\left(\frac{\partial^2\psi/\partial\varepsilon\partial\varphi}{\partial^2\psi/\partial\varepsilon^2}\right)\frac{\partial\varphi}{\partial x}\ . \tag{23}$$

Substituting (23) in the 1-d form of (19), one obtains

$$\dot{\varphi}=\frac{\partial}{\partial x}\left[\ B\left\{\ \frac{\partial^2\psi}{\partial\varphi^2}\ \ -\ \ \frac{\left(\partial^2\psi/\partial\varepsilon\partial\varphi\right)^2}{\partial^2\psi/\partial\varepsilon^2}\ \right\}\frac{\partial\varphi}{\partial x}\ \right]+s. \tag{24}$$

Consider a (hypothetical) free energy function of the form

$$\psi(\varepsilon,\varphi)=\begin{cases}\dfrac{1}{2}E\varepsilon^2(1-\varphi) & \text{for } \varepsilon<\varepsilon_0\ll 1 \text{ or } \varphi<\varphi_0\ll 1\\ E\varepsilon_m^2\left[\varphi\left(1-\ln\left(1-\varphi_m\right)\right)+(1-\varphi)\ln(1-\varphi)-\left(\varphi_m+\ln\left(1-\varphi_m\right)\right)\right] & \\ +\dfrac{1}{2}E\varepsilon^2(1-\varphi) & \text{for } \varepsilon\geq\varepsilon_0 \text{ and } \varphi\geq\varphi_0,\end{cases} \tag{25}$$

where E is the Young's modulus, $0<\varepsilon_0\ll 1,\varphi_0\ll 1$ are small thresholds below which the conventional local theory is assumed valid and in this regime we consider $B\equiv 0$. $\varepsilon_m>0,\varphi_m>0$ are two other parameters indicative of the maximum achievable strain and maximum achievable porosity. The free energy function is discontinuous at the physically insignificant small values of strain and porosity where the generalized damage model is not required. Nevertheless, the limiting values, from either side of these boundaries in $\varepsilon-\varphi$ space, of the stress, the modulus and the derivative of the stress with respect to porosity coincide. Also, the expressions for the stress and the elastic modulus corresponding to this free energy function are classical and the damage driving force $-\partial\psi/\partial\varphi>0$.

Substituting this choice (25) of the free energy function in (24) and using (23), one obtains the following governing equations:

$$\begin{aligned}&\frac{\partial}{\partial x}\left(E(1-\varphi)\frac{\partial u}{\partial x}\right)=0\\ &\dot{\varphi}=\frac{BE}{(1-\varphi)}\left(\varepsilon_m^2-\varepsilon^2\right)\frac{\partial^2\varphi}{\partial x^2}+\frac{3BE}{(1-\varphi)^2}\left(\left(\frac{\varepsilon_m}{\sqrt{3}}\right)^2-\varepsilon^2\right)\left(\frac{\partial\varphi}{\partial x}\right)^2+s.\end{aligned} \tag{26}$$

An adequate minimal requirement of the source is that it be a positive function with the sign of $\left(-\partial\psi/\partial\varphi\right)$. For the constitutive choice (25), this sign is always positive. A choice following linear kinetics for the model (25) would be

$$s=\begin{cases}D(1/2)E\varepsilon^2 & \text{for } \varphi<\varphi_0\\ DE\left(\varepsilon_m^2\ln\left(\dfrac{1-\varphi}{1-\varphi_m}\right)+(1/2)\varepsilon^2\right) & \text{for } \varphi\geq\varphi_0\end{cases} \tag{27}$$

where $D>0$ is a material parameter.

For $Dl^2 \gg B$, where l is a characteristic length in the problem (say, the length of the bar), the source term would dominate and the gradient terms would constitute singular perturbations in (26). Interestingly, the linearization of (26) suggests that the mechanical coupling provides a destabilizing influence through the diffusion term of $(26)_2$ but a void-closure effect through the nonlinear advection term. However, this linearized void-closing effect (i.e. porosity decrease at a fixed spatial location through which the void-solid interface passes) would have to compete with the more powerful positive source term thus resulting in a net increase in porosity (at fixed location).

When the source term is dropped in $(26)_2$ and the equation considered to be one with constant coefficients of the form

$$\frac{\partial \varphi}{\partial t} - \left(\frac{\partial \varphi}{\partial x} \right)^2 = \nu \frac{\partial^2 \varphi}{\partial x^2}, \quad \nu > 0, \tag{28}$$

an analytical solution becomes immediately available through the Hopf-Cole transformation for Burgers equation

$$\frac{\partial u}{\partial t} - \frac{\partial u^2}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \;\; ; \;\; \varphi_x = u \tag{29}$$

given by

$$\varphi = \nu \log w, \tag{30}$$

that reduces (28) to the linear heat equation

$$\frac{\partial w}{\partial t} = \nu \frac{\partial^2 w}{\partial x^2}. \tag{31}$$

The solution to (28) on the entire real line, when appended with the initial condition $\varphi(x,0) = \varphi_0(x)$, is given by

$$\varphi(x,t) = \nu \log \left[\frac{1}{2\sqrt{\pi \nu t}} \int_{-\infty}^{\infty} e^{(\varphi_0(y)/\nu)} e^{-(x-y)^2/4\nu t} \, dy \right], \tag{32}$$

utilizing the fundamental solution of the linear heat equation (cf. Strang, 1986). The solution (32) makes clear the role of $\nu > 0$ even in this semilinear setting.

Interestingly, for free energy functions for which the constant-coefficient version of (24) (without source) may be stated as (28) with $\nu \ll 1$, the asymptotics of (32) can be explicitly evaluated for $\nu \to 0$, coinciding with the remarkable Hopf-Lax solution formula (Lax, 1973) for the entropy-weak solution of the corresponding Hamilton-Jacobi equation (i.e. (28) with $\nu = 0$):

$$\varphi(x,t) = \max_y \left[\varphi_0(y) - \frac{(x-y)^2}{4t} \right]. \tag{33}$$

For the initial condition

$$\varphi(x,0) = H(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \tag{34}$$

The solution is given by

$$\varphi(x,t) = \max_y \left[\begin{matrix} 0(y \le 0) \\ 1(y > 0) \end{matrix} - \frac{(x-y)^2}{4t} \right] = \begin{cases} 1 & x > 0 \\ 1 - x^2/4t & -2\sqrt{t} < x < 0 \\ 0 & x < -2\sqrt{t} \end{cases}. \tag{35}$$

The initial condition may be thought of as a semi-infinite ‘crack in 1-d’ and the time evolution, represented by the schematic in Figure 1, represents the development of damage zone ahead of

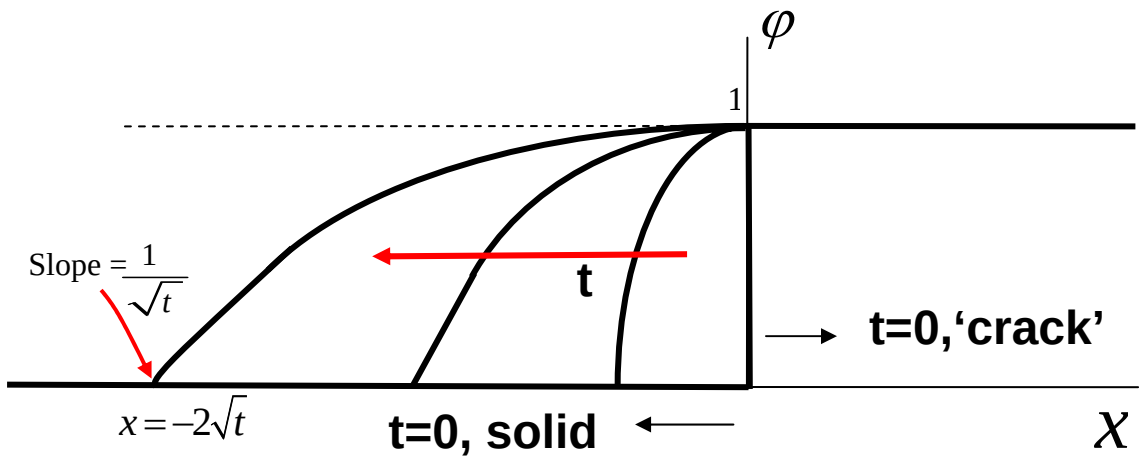

Figure 1. Schematic of solution (35) representing the development of a damage zone.

the ‘crack’ tip developing into a full-crack at long times. In the presence of the source term, this transition to a fully-voided state at fixed location may be expected to be much more rapid.

5. Discussion

It is an easy observation of some consequence that standard thermodynamic formalism with the free energy of the form (12) but without the balance law (11) yields only a local evolution equation. Even when augmented by a surface energy term, the two formalisms (with and without the balance law) yield different PDE for void volume fraction evolution. That such balance laws are not always available for any internal variable one can think of is appreciated by considering the case of plastic slip. While in the general nonlinear setting plastic distortion does enter the free energy function more than linearly, it is not immediately obvious as to how one could interpret slip as a (volume, areal) density so as to be able to write a corresponding balance law for it. However, it is possible to interpret the Nye dislocation density tensor as an areal density and therefore write a balance law for it. Of course, in this case one has to be careful in prescribing the dependence of the free energy on the dislocation density, as discussed in Sec. 2.

There remains much work to be done on identifying proper constitutive equations/parameters for this generalized model of damage. For instance, porosity spreads in highly anisotropic fashion in most real materials; this may necessitate the parameter B to be a non-hydrostatic second order tensor. As well, homogenization questions of the governing PDE are important for understanding macroscopic, nonlocal/generalized models of damage evolution.

In the present context, the most important physical question remains as the establishment of accurate free energy functions as a function of porosity (that may be accessible numerically through computational homogenization), for the entire range of admissible porosity values. If for physically rigorous free energy functions the term

$$\frac{\partial^2\psi}{\partial\varphi^2} \quad - \quad \frac{\partial^2\psi}{\partial\varphi\partial\boldsymbol{\varepsilon}} : \left(\frac{\partial^2\psi}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}\right)^{-1} : \frac{\partial^2\psi}{\partial\varphi\partial\boldsymbol{\varepsilon}} \tag{36}$$

fails to remain non-negative, then a surface energy modification has to be introduced into the free energy resulting in a fourth-order Cahn-Hilliard equation coupled to the deformation for the evolution of porosity.

In view of (36)/(24), a precise question may be phrased for determining the class of mathematically admissible free energy functions, members of which can then be subjected to elimination based on physical grounds. Explicitly (and writing the condition in the 1-d setting for simplicity), one asks for all possible appropriately smooth solutions $\psi(\varepsilon,\varphi)$ to the interesting nonlinear, 2nd-order, partial differential inequality,

$$\frac{\partial^2\psi}{\partial\varphi^2} \quad - \quad \frac{\left(\partial^2\psi/\partial\varepsilon\partial\varphi\right)^2}{\left(\partial^2\psi/\partial\varepsilon^2\right)} \geq 0 \tag{37}$$

on the domain (ε,φ) belonging to $[-\varepsilon_m,\varepsilon_m]\times[0,1]$ subject to the constraints

$$\begin{aligned}
&\psi(\varepsilon,\varphi=0)=\frac{1}{2}E\varepsilon^2,\\
&\psi(\varepsilon,\varphi=1)=0,\\
&\psi(\varepsilon=0,\varphi)=0,\\
&\frac{\partial^2\psi}{\partial\varepsilon^2}(\varepsilon,\varphi)>0 \quad \text{(modulus is positive)},\\
&\frac{\partial^2\psi}{\partial\varepsilon\partial\varphi}\neq 0 \quad \text{(damage is coupled to stress)}.
\end{aligned} \tag{38}$$

Finally, the question of what balance equation adequately represents balance of mass in this model needs to be considered in detail since the mass content of a fixed set of particles forming a subpart of the body in this model, in contrast to standard continuum mechanics, does not remain fixed in time. However, the model conceptually allows the consideration of continuous motion of a 'body' a subpart of which may have no mass as a limiting situation, and this has the potential of relieving some of the technical difficulties of classical continuum mechanics at the kinematical level in dealing with the topology change associated with material voiding/cracking.

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