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STABILITY AND ENERGY MINIMIZATION IN ELASTICITY WITH DAMAGE

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Abstract—We consider the energy minimization problem for elastic bars with continuous damage, where damage evolution is a function of strain evolution. Free energies with penalization terms are shown to be compatible with the Clausius–Duhem inequality.

For free energies with and without penalization we show that minimizers of the total free energy must be states where damage evolution vanishes.

1. INTRODUCTION

The view that the forming of macrocracks is the result of a loss of stability of a continuous damage field has gained wider acceptance in recent years (Lemaitre, 1986). Structures can accommodate moderate damage fields without failing (what moderate means depends on the particular case). Although a great amount of progress was made in this direction, we are still not close to a complete understanding of the passage from continuous damage to fracture. There may not be a unique answer: ductile damage and fragile damage may lead to fracture by different mechanisms and the key to understanding each case may be different.

The problem that interests us here is that of the stability of damaged states. With this question in mind we shall be mainly concerned with the energy minimization problem for a one-dimensional bar.

We shall begin by describing the basic mechanics of the problem, that is the type of evolution laws for damage and the stress–strain relations that we take for experimental, and therefore immutable facts. We shall consider elastic materials, not necessarily linear, where damage evolution is proportional to strain evolution.

In Section 3 we shall review the argument that leads from the Clausius–Duhem inequality to the well known thermodynamic relations between the energy, entropy and stress functions.

Our first important observation is that a free energy function—more general in form than the one normally derived—is still compatible with the Clausius–Duhem inequality. This will be called a free energy with penalization.

In Section 4 we shall look at the energy minimization problem for free energy functions without penalization and introduce for Section 5 the consideration of penalization terms. In Sections 4 and 5 we show that minimizers of the total energy cannot be states where damage evolution is possible. That is, there are states where damage evolution is possible and these are disjoint from states of admissible equilibria. This we shall argue is in agreement with the phenomenon of stress accommodation seen in traction experiments. In Section 5 we also show how a relation might be established between the penalization function and the evolution law for damage.

2. DAMAGE MECHANICS

Working conditions may alter the structure of a given material and consequently its behavior. Frequently this alteration in structure consists in the appearance of microvoids or microcracks. These can be described by a continuous damage field which measures their density (Lemaitre and Chaboche, 1985). The amount of damage at each point then evolves as a consequence of the continuing thermomechanical working. The law that governs this evolution is a characteristic of each material and each type of damage. Damage is an

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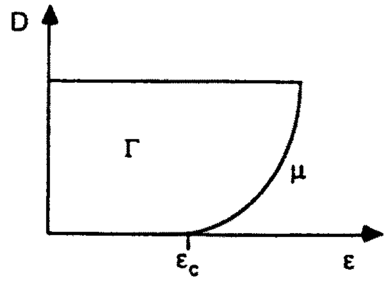

Fig. 1. Damage evolution curve on the ε, D plane.

irreversible process (at least we shall consider it to be so); thus, the time derivative of the damage variable must be positive (or zero).

In this work we shall consider damage evolution laws of the following type:

$$\dot{D} = g(\varepsilon^*, D)\langle \dot{\varepsilon}^* \rangle \tag{1}$$

where D denotes a scalar measure of damage, ε^* is a scalar measure of deformation, g is a positive function, $\langle x \rangle = \max\{x, 0\}$ and a superposed dot denotes a time derivative.

In one-dimensional problems ε^* is equal to the diplacement gradient ε. We shall normalize D so that it stays between 0 and 1.

In one-dimensional problems for monotone evolutions of deformation, (1) leads to the differential equation

$$\mathrm{d}D = g(\varepsilon, D)\,\mathrm{d}\varepsilon \tag{2}$$

whose integral we shall assume to exist and be given in the form of a monotone function

$$D = G(\varepsilon)$$

$$G(\varepsilon_c) = 0. \tag{3}$$

The critical value ε_c is the strain at which damage evolution begins.

The set $P_g = \{(\varepsilon, D) | g(\varepsilon, D) > 0\}$ is the set of the ε, D plane where $\dot{D} > 0$ if $\dot{\varepsilon} > 0$. Let Γ be the region enclosed by the graph of G and the lines $\varepsilon = 0$, $D = 0$ and $D = 1$. We have the following possibilities for P_g.

(I) $P_g = \Gamma$. In this case $\dot{D} > 0$ whenever $\dot{\varepsilon} > 0$.

(II) $P_g = \mu =$ the graph of G. In this case damage increases only along the curve μ, and there is a (trivially) convex set

$$\{\varepsilon | 0 \leqslant \varepsilon \leqslant G^{-1}(D)\}$$

which governs the evolution of damage.

(III) $\mu \subset P_g \subset \Gamma$, i.e. D evolves on a "fat" set to the left of μ in Fig. 1.

In Figs 2–4 we show examples of possible evolutions of (D, ε) indicated by the arrows. In these figures we have drawn Γ (the set under μ) convex. We shall assume that to be always the case.

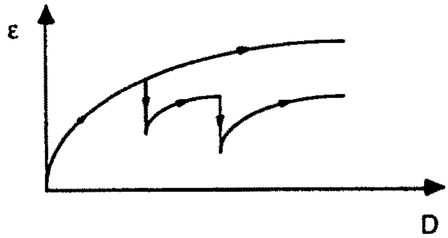

Fig. 2. Two evolution curves for type I. One is monotone and follows the curve μ and the other has two points of discharge.

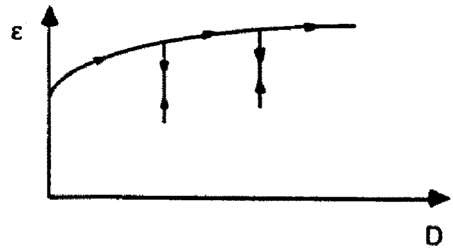

Fig. 3. Same as above for type II.

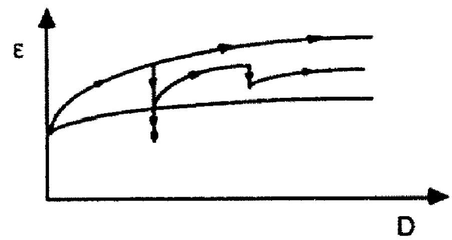

Fig. 4. Same as above for type III.

Example. If

$$g = \varepsilon/(1-D)$$

then

$$\mathrm{d}D = g\,\mathrm{d}\varepsilon$$

gives

$$\varepsilon = G^{-1}(D) = \sqrt{(2D-D^2)}+\varepsilon_c$$

which gives a convex set Γ.

Remark. The function g determines a vector field on the (D, ε) plane along which D and ε evolve.

Example. Type III (see Fig. 5). Similar figures can be drawn for types I and II.

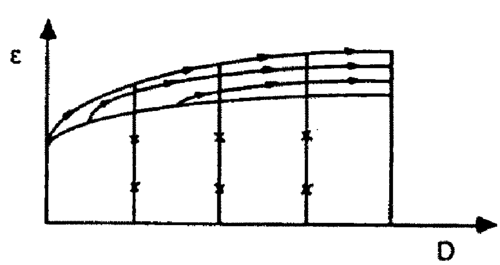

Fig. 5. (D, ε) evolution follow the arrows. Starred lines are two way.

Stress–strain relations

In our choice for a constitutive relation we shall consider only elastic materials. Letting σ denote the stress we shall assume that

$$\sigma(\varepsilon, D) = E(D)\varepsilon^r \qquad r > 0. \tag{4}$$

Here $E(D)$ denotes the modulus of elasticity; as a function of damage it satisfies

$$E'(D) < 0$$
$$E(1) = 0.$$

In many applications one can take

$$\sigma(\varepsilon, D) = E_0(1-D)\varepsilon$$

characterizing a linear elastic material with effective stress σ_e (Lemaitre and Chaboche, 1985),

$$\sigma_e = \sigma/(1-D).$$

3. DAMAGE THERMODYNAMICS

The actual thermodynamical evolution of a system must satisfy the laws of thermodynamics. Since this must hold for any subsystem, on regions where the fields defining the thermodynamical process are smooth, one can derive the so-called local forms of these laws. A combination of the first law (where the kinetic energy term is cancelled through momentum balance) with the second law yields the Clausius–Duhem inequality

$$\rho\dot{\Phi}+\rho S\dot{T}-\sigma:\dot{\varepsilon}+(1/T)\ \mathrm{grad}\ T\cdot q \leqslant 0. \tag{5}$$

Here ρ is the mass density, Φ is the Helmholtz free energy, S is the entropy, T is the temperature, $\mathrm{grad}T$ is the temperature gradient and q is the heat flux vector.

Suppose now that Φ, S, σ and q are differentiable functions of ε, T, D and $\mathrm{grad}T$; then using the chain rule on $\dot{\Phi}$ and (5), we get

$$\rho(\partial\Phi/\partial T+S)\dot{T}+(\rho\ \partial\Phi/\partial\varepsilon-\sigma):\dot{\varepsilon}+\rho\ \partial\Phi/\partial D\ \dot{D}+1/T\ \mathrm{grad}T\cdot q$$
$$+\rho\ \partial\Phi/\partial\mathrm{grad}T\ \mathrm{gr\dot{a}d}T \leqslant 0. \tag{6}$$

If ε, T, D, $\mathrm{grad}T$ and their time derivatives can be chosen independently, one can show (Coleman and Noll, 1963) that the following relations must hold.

$$\partial\Phi/\partial T\,(\varepsilon, T, D) = -S(\varepsilon, T, D)$$
$$\rho\ \partial\Phi/\partial\varepsilon\,(\varepsilon, T, D) = \sigma(\varepsilon, T, D)$$
$$\partial\Phi/\partial\mathrm{grad}T\,(\varepsilon, T, D) = 0$$
$$\partial\Phi/\partial D\,(\varepsilon, T, D) \leqslant 0 \tag{7}$$

and

$$\mathrm{grad}T\,q \leqslant 0.$$

On the other hand, in the problem that interests us $\dot{D}$ and $\dot{\varepsilon}$ are not independent since they must satisfy (1). In this case eqns (7) are still sufficient for (6) to hold for all processes; but they are no longer necessary.

Indeed, if $\dot{\varepsilon} \leqslant 0$, $\dot{T} = 0$ and $\mathrm{grad}T = 0$

$$\rho\ \partial\Phi/\partial\varepsilon-\sigma \geqslant 0 \tag{8}$$

and if $\dot{\varepsilon} \geqslant 0$, $\dot{T} = 0$ and $\operatorname{grad} T = 0$,

$$\rho\ \partial\Phi/\partial\varepsilon-\sigma+\rho g\ \partial\Phi/\partial D \geqslant 0. \tag{9}$$

Combining (8) and (9)

$$0 \leqslant \rho\ \partial\Phi/\partial\varepsilon-\sigma \leqslant -\rho g\ \partial\Phi/\partial D. \tag{10}$$

In particular, since $g \geqslant 0$,

$$\partial\Phi/\partial D \leqslant 0.$$

When $g = 0$, (8) and (10) yield the usual $(7)_2$, but on $P_g = \{(\varepsilon, D)|g(\varepsilon, D) > 0\}$, (10) may be satisfied non trivially.

For instance we may have

$$\Phi(\varepsilon, D) = \bar{\Phi}(\varepsilon, D)+h(\varepsilon, D)$$

with

$$\rho\ \partial\bar{\Phi}/\partial\varepsilon = \sigma$$

as long as the function h satisfies

$$\{(\varepsilon, D)|h(\varepsilon, D) > 0\} = P_g.$$

The function h will be called in this work a penalization term.

Example. With

$$g(\varepsilon, D) \equiv 1,$$

$$\Phi(\varepsilon, D) = E/2(1-D)\varepsilon^2+(E\ \mathrm{e}^{-D}\varepsilon^3)/6$$

and

$$\sigma = \rho E(1-D)\varepsilon$$

give

$$-\rho\ \partial\Phi/\partial D = \rho(\varepsilon^2/2+\mathrm{e}^{-D}\varepsilon^3/6)E \geqslant \rho E\ \mathrm{e}^{-D}\varepsilon^2/2 = \rho\ \partial\Phi/\partial\varepsilon-\sigma \geqslant 0.$$

4. ENERGY MINIMIZATION WITHOUT PENALIZATION

In this section we shall consider the energy minimization problem for a one-dimensional bar with damage and with the free energy function

$$\Phi(\varepsilon, D) = \int \sigma(\varepsilon, D)\ \mathrm{d}\varepsilon = E(D)\varepsilon^{r+1}/(r+1).$$

Throughout we shall take for granted that equilibrium states are those for which the total free energy—including that of the external loads—is stationary, and that minimizers of this energy are stable (locally if the minimizer is local).

Consider a one-dimensional bar of length L whose deformed length λ is imposed. In an isothermal situation one looks for minimizers of

$$\mathscr{E}[\varepsilon, D] = \int_0^L \bar{\rho}\Phi(\varepsilon, D)\, \mathrm{d}x \tag{11}$$

among all states $(\varepsilon, D) : [0, L]\ R^+ \times [0, 1]$ such that

$$\int_0^L \varepsilon\, \mathrm{d}x = \lambda.$$

In (11), $\bar{\rho}$ is the reference density.

Suppose now that there exists a minimizer $(\bar{\varepsilon}, \tilde{D})$ of $\mathscr{E}$ and let us take a variation $\delta\varepsilon = \omega(x)$ satisfying the constraint

$$\int_0^L \omega\, \mathrm{d}x = 0. \tag{12}$$

Let

$$L_+ = \{x \in [0, L] \mid \omega(x) > 0\}$$
$$L_- = \{x \in [0, L] \mid \omega(x) \leqslant 0\}.$$

Thus, L_+ and L_- are the parts of the bar where the deformation is increased and decreased, respectively.

Then

$$\delta\mathscr{E}[\bar{\varepsilon}, \tilde{D}]\omega = \int_{L_+} \{\bar{\rho}\ \partial\Phi/\partial\varepsilon\ (\bar{\varepsilon}, \tilde{D}) + \bar{\rho}\ \partial\Phi/\partial D\ (\bar{\varepsilon}, \tilde{D})g(\bar{\varepsilon}, \tilde{D})\}\omega\, \mathrm{d}x + \int_{L_-} \bar{\rho}\ \partial\Phi/\partial\varepsilon\ (\bar{\varepsilon}, \tilde{D})\omega\, \mathrm{d}x \tag{13}$$

since $\delta D = 0$ if $\delta\varepsilon \leqslant 0$, and $\delta D = g\omega$ in L_+.

If we take

$$\omega(x) = u(x) - (1/L)\int_0^L u\, \mathrm{d}x$$

for arbitrary u, evidently ω satisfies (12). Then, after changing orders of integration, (13) can be written as

$$\delta\mathscr{E}[\bar{\varepsilon}, \tilde{D}]u = \int_0^L \left\{H(x) - \int_0^L H(\xi)\, \mathrm{d}\xi\right\}u(x)\, \mathrm{d}x$$

where

$$H(x) = \begin{cases} \bar{\rho}\ \partial\Phi/\partial\varepsilon\ (\bar{\varepsilon}(x), \tilde{D}(x)) + \bar{\rho}\ \partial\Phi/\partial D\ (\bar{\varepsilon}(x), \tilde{D}(x))g(\bar{\varepsilon}(x), \tilde{D}(x)) & \text{if } x \in L_+ \\ \bar{\rho}\ \partial\Phi/\partial\varepsilon\ (\bar{\varepsilon}(x), \tilde{D}(x)) & \text{if } x \in L_-. \end{cases}$$

If $(\bar{\varepsilon}, \tilde{D})$ is a minimizer

$$\delta\mathscr{E}[\bar{\varepsilon}, \tilde{D}]u \geqslant 0$$

for any u integrable on $[0, L]$. That is, using a classical lemma in the Calculus of Variations,

$$H(x) \geqslant (1/L) \int_0^L H(\xi)\, d\xi$$

which in turn implies

$$H(x) = (1/L) \int_0^L H(\xi)\, d\xi = C$$

since a function cannot be greater than its average everywhere. Therefore

$$\bar{\rho}\, \partial\Phi/\partial\varepsilon\, (\bar{\varepsilon}, \tilde{D}) + \bar{\rho}\, \partial\Phi/\partial D\, (\bar{\varepsilon}, \tilde{D}) g(\bar{\varepsilon}, \tilde{D}) = C \qquad \text{on } L_+ \tag{14a}$$

and

$$\bar{\rho}\, \partial\Phi/\partial\varepsilon\, (\bar{\varepsilon}, \tilde{D}) = C \qquad \text{on } L_- \tag{14b}$$

must hold.

If we take now $\delta\varepsilon = -\omega$, L_+ and L_- change places. Since the constant C depends only on the pair of functions $(\bar{\varepsilon}, \tilde{D})$, (14) implies that

$$\partial\Phi/\partial D\, (\bar{\varepsilon}, \tilde{D}) g(\bar{\varepsilon}, \tilde{D}) = 0.$$

Thus, unless $(\bar{\varepsilon}, \tilde{D})$ takes a value where $\partial\Phi/\partial D = 0$, minimizers of the total energy must be at points were $g = 0$; that is where $\delta D = 0$ for any (small) $\delta\varepsilon$ positive or negative. In particular if evolution is of type I, *no state* may be a minimizer of the energy!

Remark. A simpler argument than the one presented above can be used if one is willing to take for granted that the mechanical equilibrium condition

$$\bar{\rho}\, \partial\Phi/\partial\varepsilon\, (\bar{\varepsilon}, \tilde{D}) = \text{const.}$$

holds everywhere. Because then it follows at once from (13) that

$$\delta\mathscr{E}[\bar{\varepsilon}, \tilde{D}]\omega = \int_{L_+} \bar{\rho}\, \partial\Phi/\partial D(\bar{\varepsilon}, \tilde{D}) g(\bar{\varepsilon}, \tilde{D})\omega\, dx$$

and since $\partial\Phi/\partial D \leqslant 0$ and $g \geqslant 0$, $\delta\mathscr{E} \geqslant 0$ if and only if $g\, \partial\Phi/\partial D = 0$. □

Damage evolution is an irreversible process. Since $\partial\Phi/\partial D \leqslant 0$, absolute minimizers of the total energy are states for which $D = 1$. But there are plenty of observable equilibria that are not *absolute* minimizers. Let us accompany the evolution of a system through a sequence of metastable equilibria: consider the problem of a one-dimensional bar in which the stress σ^* at one end is controlled and let us accompany the evolution of the bar as σ^* varies. For a sequence of equilibria, each state must satisfy the mechanical equilibrium condition

$$\sigma(x) \equiv \sigma^*.$$

That is,

$$E(D(x))\varepsilon^r(x) = \sigma^*$$

or

$$\varepsilon(x) = [\sigma^*/E(D(x))]^{1/r}. \tag{15}$$

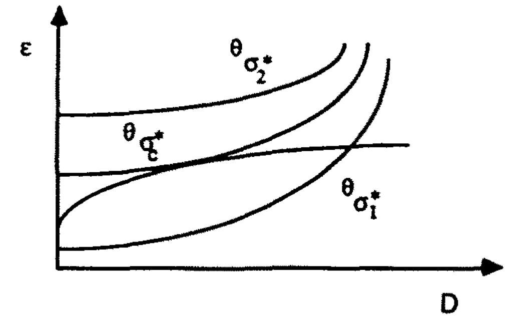

Fig. 6. Damage evolution at constant stress.

For given σ^*, equilibrium states must lie on the curve θ_{σ^*} in the ε, D plane, defined by

$$\varepsilon = [\sigma^*/E(D)]^{1/r}. \tag{16}$$

An easy computation shows that $E'(D) < 0$ and $E''(D) < 0$ imply that $\varepsilon'(D) > 0$ and $\varepsilon''(D) > 0$ if $r > 0$.

Example. In the linear case

$$\sigma = E_0(1-D)\varepsilon$$

and

$$\varepsilon = E_0\sigma^*/(1-D).$$

Thus, $\varepsilon'(D) > 0$ and $\varepsilon''(D) > 0$ as is easily verified.

Let us now plot the curve θ_{σ^*} defined by (16) with the curve μ defined by (3) (see Fig. 6).

Suppose that damage evolution is of type II, that is damage evolves only along the curve μ and that Γ (the region below μ) is convex. Any state in Γ can be attained following the evolution law. States above μ cannot be attained. Thus, there is a critical value of stress σ_c above which there is no solution satisfying mechanical equilibrium. This is well in agreement with the softening phenomenon found in experiments.

For $\sigma^* = \sigma_c$, the curves θ_{σ^*} and μ are tangent at their (single) intersection point, which lies on P_q. We have seen that such a point cannot be a minimizer of the total energy for imposed length and is, therefore, unstable. To see that it is also unstable under imposed external load, let us look at the free energy of the system including that of the external loads

$$\mathscr{F}[\varepsilon, D] = \int_0^L \{\bar{\rho}\Phi(\varepsilon, D) - \sigma^*\varepsilon\}\, \mathrm{d}x.$$

Suppose $\tilde{\varepsilon}$, $\tilde{D}$ is a minimizer of $\mathscr{F}$. Then, with the same notation as in (13),

$$\delta\mathscr{F}[\tilde{\varepsilon}, \tilde{D}]\omega = \int_{L_+} \{\bar{\rho}\, \partial\Phi/\partial\varepsilon\, (\tilde{\varepsilon}, \tilde{D}) + \bar{\rho}\, \partial\Phi/\partial D\, (\tilde{\varepsilon}, \tilde{D})g(\tilde{\varepsilon}, \tilde{D}) - \sigma^*\}\omega\, \mathrm{d}x$$
$$+ \int_{L_-} \{\bar{\rho}\, \partial\Phi/\partial\varepsilon\, (\tilde{\varepsilon}, \tilde{D}) - \sigma^*\}\omega\, \mathrm{d}x$$

for arbitrary ω.

Therefore we get (14) with σ^* replacing C and the same conclusion follows, namely that minimizers must satisfy

$$\partial\Phi/\partial D\ (\tilde{\varepsilon},\tilde{D})g(\tilde{\varepsilon},\tilde{D}) = 0.$$

Since for the cases we consider here

$$\Phi(\varepsilon, D) = E(D)\varepsilon^{r+1}/(r+1)$$

and we assumed that

$$E(D) < 0$$

and

$$\partial\Phi/\partial D < 0,$$

points in P_a cannot be stable under applied external loads.

The derivative of Φ along the curve θ_{σ^*} defined by (16) is

$$\begin{aligned} \mathrm{d}\Phi/\mathrm{d}D &= \partial\Phi/\partial\varepsilon\ \mathrm{d}\varepsilon/\mathrm{d}D + \partial\Phi/\partial D \\ &= -(E'(D)\varepsilon^{r+1})/r(r+1) > 0. \end{aligned} \tag{17}$$

Thus, for fixed stress, the free energy is smallest when D is smaller.

On the other hand

$$\mathrm{d}(\bar{\rho}\Phi - \varepsilon\sigma^*)/\mathrm{d}D = (\bar{\rho}\ \partial\Phi/\partial\varepsilon - \sigma^*)\ \mathrm{d}\varepsilon/\mathrm{d}D + \partial\Phi/\partial D < 0. \tag{18}$$

since

$$\rho\ \partial\Phi/\partial\varepsilon = \sigma = \sigma^*$$

and

$$\partial\Phi/\partial D < 0.$$

Therefore, for fixed stress, the total free energy of the system is smaller for larger D. This, though, does not imply that a state on θ_{σ^*} is necessarily unstable. This will only be the case on parts of θ_{σ^*} where $g > 0$.

If $g > 0$ only on μ, the states nearer to it are less stable since it takes smaller perturbations to bring them to a point (in μ) where they can evolve to states of smaller energy.

If a state (ε, D) is in θ_{σ^*} it satisfies the Euler–Lagrange necessary condition $\sigma^* = \sigma$ for a minimizer. Further necessary and sufficient conditions have to be met to make that state a minimizer (local of global). Global minima cannot be found since (18) holds along the states that satisfy this necessary condition. The state on this curve that has the smallest value of $\bar{\rho}\Phi - \varepsilon\sigma^*$ is unstable since it lies on μ a region of possible damage evolution. A local minimizer $(\tilde{\varepsilon}, \tilde{D})$, on the other hand, is only required to satisfy

$$\bar{\rho}\Phi(\tilde{\varepsilon}, \tilde{D}) - \tilde{\varepsilon}\sigma^* \leqslant \bar{\rho}\Phi(\varepsilon, D) - \varepsilon\sigma^* \tag{19}$$

for any ε, D in an admissible neighborhood; that is, for states that are near *along the possible curves of evolution.*

For a state where $g = 0$, (19) must hold for all ε near to $\tilde{\varepsilon}$.

Thus, a state $(\tilde{\varepsilon}, \tilde{D})$ is a (strict) local minimizer of $\mathcal{F}[\varepsilon, D]$ if its image is on the curve θ_{σ^*}—strictly below μ—and

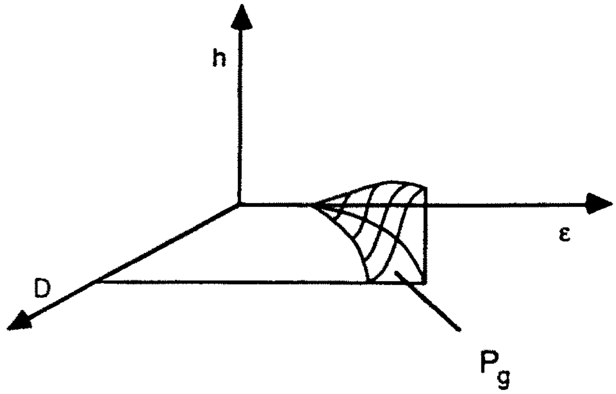

Fig. 7. An example of a penalization function.

$$\partial^2\Phi/\partial^2\varepsilon\ (\bar{\varepsilon}, \tilde{D}) \geqslant 0.$$

The convexity of Φ in ε and D is not relevant. Note that

$$\partial^2\Phi/\partial^2\varepsilon = rE(D)\varepsilon^{r-1}.$$

Conclusion. For a free energy function without penalization, an evolution law for damage of type I is thermodynamically inconsistent since no equilibrium state is a local minimizer of the total free energy.

For an evolution law of type II, states whose image lie on the curve of evolution μ cannot be minimizers. Any state in $0_{\sigma^*} \cap \{g = 0\}$ may be a relative minimizer, but not an absolute one. The state of the system must be determined from the evolution. Non-homogeneous initial data for damage will lead to non-homogeneous local minimizers.

Similar considerations hold for evolutions of type III.

Since evolution must occur along μ (type II), but there are no equilibrium states on this curve, the actual evolution of a system will show at every rest point a small accommodation corresponding to the motion of the system to a nearby stable state.

5. THE MINIMUM PROBLEM FOR A FREE ENERGY WITH PENALIZATION

We have seen in Section 3 that a free energy function of the form

$$\Phi(\varepsilon, D) = \bar{\Phi}(\varepsilon, D) + h(\varepsilon, D)$$

with

$$\bar{\rho}\ \partial\bar{\Phi}/\partial\varepsilon = \sigma$$

is compatible with the Second Law of Thermodynamics if

$$\partial h/\partial\varepsilon \geqslant 0 \tag{20}$$

and

$$\partial h/\partial\varepsilon + g\ \partial h/\partial D \leqslant -g\ \partial\Phi/\partial D \qquad \text{if } g > 0. \tag{21}$$

Where $g = 0$ we must have $h = 0$.

For damage evolution of type II where $g \neq 0$ only on a curve μ, the condition $g = 0 \Rightarrow h = 0$ requires h to be either identically zero or discontinuous. The first case was already considered and the second violates the hypothesis of differentiability of Φ used in the derivation of (20) and (21). Here we shall simply say that a free energy with penalization is incompatible with damage evolution of type II instead of reconsidering the Clausius–Duhem inequality for discontinuous Φ.

Suppose now that g is continuous. Then P_g has a nonempty interior, and in this set (20) and (21) hold (Fig. 7).

We now suppose that

$$\mathscr{F}[\varepsilon, D] = \int_0^L \{\bar{\rho}\Phi(\varepsilon, D) + \bar{\rho}h(\varepsilon, D) - \sigma^*\varepsilon\} \, dx$$

has a minimizer $\tilde{\varepsilon}$, $\tilde{D}$. Then, with the notation of (13) and $\tilde{\bar{\Phi}} = \Phi(\tilde{\varepsilon}, \tilde{D})$ etc., it must satisfy

$$\delta\mathscr{F}[\tilde{\varepsilon}, \tilde{D}]\omega = \int_{L_+} \{\bar{\rho}\, \partial\tilde{\bar{\Phi}}/\partial\varepsilon + \bar{\rho}\, \partial\tilde{\bar{h}}/\partial\varepsilon + \bar{\rho}\tilde{g}\, \partial\tilde{\bar{\Phi}}/\partial D + \bar{\rho}\tilde{g}\, \partial\tilde{\bar{h}}/\partial D - \sigma^*\}\omega \, dx$$

$$+ \int_{L_-} \{\bar{\rho}\, \partial\tilde{\bar{\Phi}}/\partial\varepsilon + \bar{\rho}\, \partial\tilde{\bar{h}}/\partial\varepsilon - \sigma^*\}\omega \, dx \leqslant 0.$$

for all integrable ω on $[0, L]$.

This yields the pointwise conditions

$$-(\bar{\rho}\, \partial\tilde{\bar{\Phi}}/\partial\varepsilon + \bar{\rho}\, \partial\tilde{\bar{h}}/\partial\varepsilon - \sigma^*) \geqslant 0$$

and

$$\bar{\rho}\, \partial\tilde{\bar{\Phi}}/\partial\varepsilon + \bar{\rho}\, \partial\tilde{\bar{h}}/\partial\varepsilon + \bar{\rho}\tilde{g}\, \partial\tilde{\bar{\Phi}}/\partial D + \bar{\rho}\tilde{g}\, \partial\tilde{\bar{h}}/\partial D - \sigma^* \geqslant 0.$$

Adding, we get

$$\bar{\rho}(\partial\tilde{\bar{\Phi}}/\partial D + \partial\tilde{\bar{h}}/\partial D)\tilde{g} \geqslant 0,$$

which is compatible with (21) if and only if $g = 0$.

We are again led to the conclusion that equilibrium occurs only at points where $g = 0$ as in the case without penalization. Thus, for the description of equilibrium states a function with penalization is indistinguishable from one without. In particular, evolutions of type I are thermodynamically inconsistent.

The only type of evolution where penalization might be of use is in evolutions of type III. Note that, since g may be strictly positive only on a narrow band around μ, in experiments it might be difficult to distinguish types II and III; specially with equilibrium measurements.

We have thus shown that free energies with penalization are compatible with thermodynamics and that in equilibrium they reduce to ordinary free energies without penalization. We conjecture that penalization might be useful in calculations where dynamics play an important role.

Remark. Above we have assumed that g is a given function; and from it we have derived restrictions on the penalization function h. One may consider that h is given and that g is (partially) determined by

$$g \geqslant \partial h/\partial\varepsilon/(-\partial h/\partial D - \partial\Phi/\partial D)$$

which comes from (21). One could, for instance, take g satisfying the relation above with equality.

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