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On damage regularity and defect nucleation modelling

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Abstract

The purpose of this article is to model defect nucleation. The defect is considered as a small volume which evolves as a damaged zone. The damage is described by a transition zone which can be sharp or continuous. In the first case, discontinuities occur and the initiation of defect is based on bifurcation of an equilibrium state. When the transition is continuous, the initiation of the defect is continuous. The analysis is based on considering different models of damage, depending on the regularity imposed on mechanical field. For each model, the presence of discontinuities on mechanical fields is investigated. Consequences of each model on defect nucleation are illustrated on particular structures: bars under extension and spheres under radial loading.

Key words: Bifurcation; Nucleation of defect; Moving interface.

1. Introduction

Fracture mechanics is generally not accurate to model the full scenario of degradation of solids under mechanical loading, damage description is more appropriate for modelling the gradual loss of stiffness.

To model defect nucleation, many approaches have been proposed. Nucleation of defect can be modelled by the appearance of a small cavity like in non-linear elasticity [1, 2, 3], in viscoplasticity [4] or in plasticity [5, 6]. J. Ball

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[1] carried out a theoretical analysis of radially symmetric cavitation in elastic solids. The results are based on comparison between the strain energy of a homogeneous sphere and those of a sphere containing an infinitesimal void at the same radial loading. This bifurcation analysis provides the critical stress, load at which the cavitation appears. Extension of this approach based on damage mechanics has been proposed in [7] for brittle materials and more recently [8] for more general damage models.

The simplest model of damage is described by a scalar function d which evolves from 0 to 1. Simultaneously the stiffness of the material is decreasing. After a critical load, uniqueness of equilibrium solution is **lost**, localization occurs. To avoid spurious localization several models were proposed in the literature : non local damage models, **higher-order** gradient models through the inclusion of deformation gradient, or damage gradient [9, 10, 11] as in phase field approach [12, 13] and in the so-called variational approach of fracture [14].

Another point of view has been developed from many years based on moving interfaces or layers. These studies emphasize the role of discontinuities in the description of damage. When the transition from a sound material to a damaged one is sharp, the evolution of damage is associated with a moving surface as in [15, 7], when the transition is more regular, the evolution of damage is associated with a moving layer [16, 17, 18].

This paper proposes a discussion of the existence of discontinuities and presents a comparison between models to predict nucleation of defect. **Influence of the regularity of the fields on the defect initiation is studied using different constitutive laws for damage modelling: a model with damage gradient as in phase-field theory [12, 19, 20], and a model with internal constraint as the thick-level-set model [16, 18].**

2. A simple local damage model

The free energy w depends on the strain ε and on a scalar damage variable d . The state laws are obtained by differentiating the free energy w with respect

to the state variables [21, 22, 23]:

$$w(\varepsilon, d), \quad \sigma = \frac{\partial w}{\partial \varepsilon}, Y = -\frac{\partial w}{\partial d}, \quad (1)$$

where σ is the local stress and Y the local energy release rate. For instance, if we consider symmetric behaviour on traction and compression, we use the potential:

$$w(\varepsilon, d) = \frac{1}{2} \varepsilon : \mathbb{C}(d) : \varepsilon. \quad (2)$$

The undamaged material has the properties $\mathbb{C}_0 = \mathbb{C}(0)$, the damaged one $\mathbb{C}_1 = \mathbb{C}(1)$. The evolution of stiffness can be described by simple forms ($\mathbb{S}_i = \mathbb{C}_i^{-1}$):

$$\begin{aligned} \mathbb{C}(d) &= \omega(d)\mathbb{C}_0 + (1 - \omega(d))\mathbb{C}_1, \\ \mathbb{S}(d) &= \omega(d)\mathbb{S}_0 + (1 - \omega(d))\mathbb{S}_1. \end{aligned} \quad (3)$$

where $\omega(d)$ is a continuous decreasing function from $\omega(0) = 1$ to $\omega(1) = 0$. When $\mathbb{C}_1 \neq \mathbf{0}$, this model describes quasi-brittle materials, and totally damaged material is obtained with $\mathbb{C}_1 = \mathbf{0}$. Such behaviours are generalizations of behaviours considered in [24]. **Function $\omega(d)$ can be a power law ($\alpha \geq 0$):**

$$\omega(d) = \frac{1}{1 + \alpha} (1 - d)^{\alpha+1}, \alpha > 0, \quad g(d) = -\omega' = (1 - d)^\alpha. \quad (4)$$

More complex functions ω have been introduced in [20, 25].

In presence of hardening, hardening function $H(d) = \int_0^d h(p) dp$ is added to free energy:

$$w_H(\varepsilon, d) = w(\varepsilon, d) + H(d), \quad (5)$$

and the local dissipation, per unit of volume, becomes:

$$D = Y_h \dot{d}, \quad Y_h = Y - h(d) = -\frac{\partial w_H}{\partial d} = \frac{g(d)}{2} \varepsilon : \mathbb{C}_0 : \varepsilon - h(d). \quad (6)$$

2.1. Evolution of damage parameter

The evolution laws is given generally in terms of a regular function $\Phi(Y, d)$:

$$\dot{d} = \frac{\partial \Phi}{\partial Y_h}. \quad (7)$$

In this presentation, a generalized standard material [23] is used; this framework ensures the positivity of the local dissipation. The driving force Y derives from a positive function $\phi(\dot{d})$ convex of \dot{d} ($\phi(\dot{d}) \geq 0$, $\phi(0) = 0$):

$$Y_h = \frac{\partial \phi}{\partial \dot{d}}. \quad (8)$$

When $\phi(\dot{d})$ is a positive homogeneous convex function of degree one, the behaviour is rate independent.

Instead of $\phi(\dot{d})$, the dual convex potential $\phi^*(Y_h)$ may be used such that

$$\phi^*(Y_h) = \sup_{\dot{d}} (Y_h \cdot \dot{d} - \phi(\dot{d})), \quad \dot{d} = \frac{\partial \phi^*}{\partial Y_h}. \quad (9)$$

For non-regular function $\phi(\dot{d})$, the differential (8) is replaced by the notion of sub-differential

$$Y_h \in \partial \phi, \quad \phi(\dot{d}) + Y_h(\dot{d}^* - \dot{d}) \leq \phi(\dot{d}^*), \forall \dot{d}^*. \quad (10)$$

Consider, the non-smooth function:

$$\phi(\dot{d}) = \begin{cases} Y_c \dot{d}, & \text{if } \dot{d} \geq 0, \\ +\infty, & \text{otherwise.} \end{cases} \quad (11)$$

The normality rule is recovered:

$$Y_h \leq Y_c, \quad \dot{d} \geq 0, \quad (Y_h - Y_c)\dot{d} = 0. \quad (12)$$

In this case, the behaviour is rate-independent. Introducing the convex set \mathcal{C} :

$$\mathcal{C} = \{Y_h | Y_h - Y_c \leq 0\}, \quad (13)$$

the normality rule is rewritten in terms of the indicator function $I_{\mathcal{C}}$ of the convex set \mathcal{C}

$$\dot{d} \in \partial I_{\mathcal{C}}, \quad I_{\mathcal{C}} = \begin{cases} 0, & \text{if } Y_h \in \mathcal{C}, \\ +\infty, & \text{otherwise.} \end{cases} \quad (14)$$

2.2. Properties of damage

With respect to normality rule (11,12), the domain Ω is decomposed into two sub-domains

$$\begin{cases} \Omega^o, & Y_h < Y_c, & \dot{d} = 0, \\ \Omega^+, & Y_h = Y_c, & \dot{d} \geq 0. \end{cases} \quad (15)$$

Any compatible variations δd of d with the normality rule are defined on the set

$$\delta d \in \mathcal{K} = \{d^* | d^* = 0 \text{ over } \Omega^o, d^* \geq 0 \text{ over } \Omega^+\}. \quad (16)$$

2.3. Models with local discontinuities : an axial description

Consider a bar, with length L , under uni-axial loading. At point $x \in [0, L]$, displacement is $\mathbf{u}(x)$. The stiffness \mathbb{C}_0 is reduced to Young's modulus E_0 . The free energy (5) with hardening is then:

$$w_H(\varepsilon, d) = \frac{1}{2}\omega(d)E_0\varepsilon^2 + \int_0^d h(p) dp. \quad (17)$$

The equilibrium solution satisfies

$$\sigma = \omega(d)E_0\varepsilon, \quad \frac{d\sigma}{dx} = 0. \quad (18)$$

then the stress is uniform $\sigma(x) = \Sigma$. The driving force Y_h becomes:

$$Y_h = \frac{g(d)}{2}E_0\varepsilon^2 - h(d). \quad (19)$$

The fundamental solution. The fundamental solution is a uniform strain ε with a uniform damage d . For $\omega = (1 - d)$ and $(1 - d)^2/2$ and different $h(d) = h_o d^\beta$ we obtain different responses illustrated on figure 1. When softening occurs, several solutions $\Delta = u(L)/L$ can appear for the same Σ . At state Σ , the bar can be decomposed into a finite number n of sub-domains $\Omega_i, i = 1 \dots n$, over each one the damage d is uniform $d(x) = d_i$. Therefore we have:

$$Y_i = \frac{1}{2}g(d_i)E_0\varepsilon_i^2 - h(d_i) \leq Y_c, \quad \sigma_i = \omega(d_i)E_0\varepsilon_i = \Sigma. \quad (20)$$

Taking account of the local damage law ω and of the hardening function $h = h_o d^\beta$, we have

$$f(d_i) = (\alpha + 1)^2 \frac{\Sigma^2}{2E_0(1 - d_i)^{\alpha+1}} - h_o d_i^\beta \leq Y_c. \quad (21)$$

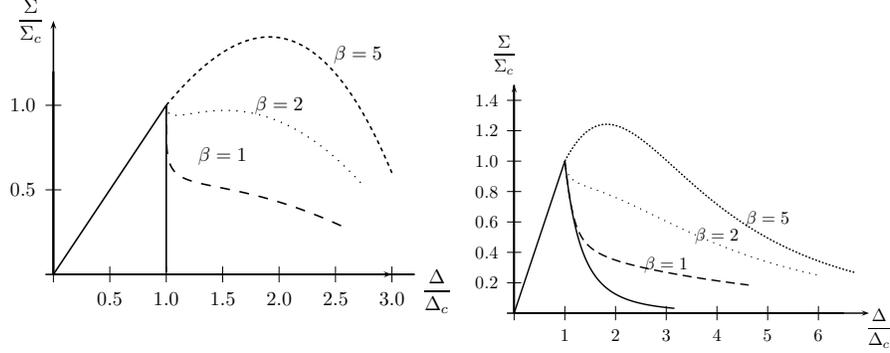


Figure 1: Homogeneous response of the bar, left : $\alpha = 0$, $h_o = 0$ and $h_o = 10$, $\beta = 1(-)$, $2(\cdot)$, $5(- -)$ right: $\alpha = 1$, $h_o = 0$ and $h_o = 10$, $\beta = 1(-)$, $2(\cdot)$, $5(- -)$.

The function f is a decreasing function of d_i , damage evolves where f is maximum, this occurs on the sub-domain Ω_m , where $d_m = \max_i d_i$. Simultaneously, when damage evolves, the stress Σ decreases and the volume Ω_m can be decomposed into two sub-domains :

$$\Omega_m^0 \text{ where } \dot{d} = 0, \quad \Omega_m^+ \text{ where } \dot{d} > 0. \quad (22)$$

This shows the multiplicity of solutions. To avoid such multiplicity more regularity is required on the damage variable.

3. Models with moving interface

We consider a surface which separates two domains with different mechanical characteristics, then mechanical fields can be discontinuous.

3.1. General features

Consider a body Ω decomposed into two sub-domains Ω_0 , Ω_1 with common boundary Γ . At a point X_Γ , the normal vector to Γ is \mathbf{n}_γ outward Ω_0 . The motion of Γ is described by the normal velocity $\mathbf{v}_n(X_\Gamma) = -a\mathbf{n}_\gamma$, (see figure 2). The material of Ω_0 is transformed into the material of Ω_1 when the interface Γ is

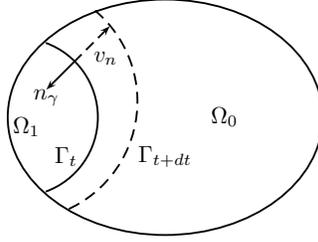


Figure 2: A moving surface : evolution of Ω_0 and Vol_1

moving with $a \geq 0$. On the surface Γ any mechanical quantity f can experience a jump denoted by

$$[[f]]_{\Gamma} = f_0 - f_1. \quad (23)$$

Any volume average has a rate defined by

$$\frac{d}{dt} \int_{\Omega(\Gamma)} f \, d\Omega = \int_{\Omega(\Gamma)} \dot{f} \, d\Omega - \int_{\Gamma} [[f]]_{\Gamma} a \, dS. \quad (24)$$

Time derivative of integrals defined on varying volume and surface domains has been investigated in [26].

Perfect bonding and discontinuities. Along the interface perfect bonding is preserved at any time. Let us introduce the convective derivative.

Convective derivation. The convective derivative D_a of any function $f(X_{\Gamma}, t)$ is

$$D_a(f) = \lim_{\tau \rightarrow 0} \frac{f(X_{\Gamma} + \mathbf{v}_n \tau, t + \tau) - f(X_{\Gamma}, t)}{\tau} \quad (25)$$

Any continuous mechanical quantity along Γ satisfies the general compatibility conditions of Hadamard rewritten in terms of convective derivative:

$$[[f]]_{\Gamma} = 0 \Rightarrow D_a([[f]]_{\Gamma}) = [[\dot{f}]]_{\Gamma} - a[[\nabla f]]_{\Gamma} \cdot \mathbf{n}_{\Gamma} = 0. \quad (26)$$

3.2. The sharp interface and moving discontinuity

The domain Ω is decomposed as a two-phase composite, sound material in domain Ω_0 with stiffness \mathbb{C}_0 and transformed material in domain Ω_1 with

stiffness \mathbb{C}_1 . The local free energy is defined on each phase as

$$\begin{cases} w_0(\varepsilon) &= \frac{1}{2}\varepsilon : \mathbb{C}_0 : \varepsilon, & \text{over } \Omega_0, \\ w_1(\varepsilon) &= \frac{1}{2}\varepsilon : \mathbb{C}_1 : \varepsilon + H, & \text{over } \Omega_1, \end{cases} \quad (27)$$

where $\varepsilon(\mathbf{u})$ is the strain. The constant $H \geq 0$ is a stored energy due to the transformation from material (0) to material (1).

The internal parameter d presents a strong discontinuity: $d_0 = 0$, over Ω_0 and $d_1 = 1$, over Ω_1 , then $[[d]]_\Gamma = -1$. At every time, bonding is perfect along the interface Γ , therefore displacement and stress vector are continuous.

3.3. The equilibrium state

We study now the equilibrium of the body Ω submitted to given boundary conditions (BC).

Boundary conditions (BC). The external boundary $\partial\Omega$ of the body Ω is decomposed into two complementary parts ($\partial\Omega = \partial\Omega_u \cup \partial\Omega_T$): on $\partial\Omega_u$ the displacement is imposed ($\mathbf{u}(x, t) = \mathbf{u}^d(x, t)$, $x \in \partial\Omega_u$) and on $\partial\Omega_T$, the traction $\mathbf{T}^d(x, t)$ is prescribed.

The unknowns of the equilibrium problem defined on Ω are displacements \mathbf{u} and position of the internal boundary Γ .

The potential energy. The total potential energy of the body is:

$$\mathcal{E}(\mathbf{u}, \Gamma) = \int_{\Omega_0(\Gamma)} w_0(\varepsilon(\mathbf{u})) \, d\Omega + \int_{\Omega_1(\Gamma)} w_1(\varepsilon(\mathbf{u})) \, d\Omega - \int_{\partial\Omega_T} \mathbf{T}^d \cdot \mathbf{u} \, dS. \quad (28)$$

The position of the interface Γ plays the role of an internal parameter.

Displacements are continuous along Γ , then velocities are satisfying the Hadamard's relations for discontinuities (26):

$$[[\mathbf{u}]]_\Gamma = 0, \quad [[\dot{\mathbf{u}}]]_\Gamma - a[[\nabla\mathbf{u}]]_\Gamma \cdot \mathbf{n}_\gamma = 0, \quad (29)$$

where $\mathbf{v}_n = -a(s) \mathbf{n}_\gamma$ is the normal velocity associated to the motion of Γ . As Γ can move, variations of displacement should be compatible with possible motion of Γ defined by δa

$$[[\delta\mathbf{u}]]_\Gamma - \delta a[[\nabla\mathbf{u}]]_\Gamma \cdot \mathbf{n}_\gamma = 0. \quad (30)$$

Any variations $\delta \mathbf{u}$ of the displacement must be also compatible with the boundary conditions (BC.3.3) : $\delta \mathbf{u}(x) = 0, x \in \partial\Omega_u$.

Variations of the potential energy. The variations of \mathcal{E} becomes:

$$\frac{\partial \mathcal{E}}{\partial \mathbf{u}} \cdot \delta \mathbf{u} + \frac{\partial \mathcal{E}}{\partial \Gamma} \delta \Gamma = \sum_{i=0,1} \int_{\Omega_i} \sigma_i : \nabla \delta \mathbf{u} \, d\Omega - \int_{\partial\Omega_T} \mathbf{T}^d \cdot \delta \mathbf{u} \, dS - \int_{\Gamma} \llbracket w \rrbracket_{\Gamma} \delta a \, dS.$$

after integration by parts, we obtain two contributions: one inside the domain and another over the surface Γ

$$\begin{aligned} \delta \mathcal{E} &= \sum_{i=0,1} \int_{\Omega_i} -\operatorname{div} \sigma_i \cdot \delta \mathbf{u} \, d\Omega - \int_{\partial\Omega} \mathbf{n} \cdot \sigma \cdot \delta \mathbf{u} \, dS - \int_{\partial\Omega_T} \mathbf{T}^d \cdot \delta \mathbf{u} \, d\Omega \\ &+ \int_{\Gamma} \mathbf{n}_{\gamma} \cdot \llbracket \sigma \cdot \delta \mathbf{u} \rrbracket_{\Gamma} \, dS - \int_{\Gamma} \llbracket w \rrbracket_{\Gamma} \delta a \, dS. \end{aligned} \quad (31)$$

Taking account of the compatibility of $\delta \mathbf{u}$ (30), two independent contributions are obtained:

$$\int_{\Gamma} \mathbf{n}_{\gamma} \cdot \llbracket \sigma \rrbracket_{\Gamma} \cdot \delta \mathbf{u}_o \, dS - \int_{\Gamma} (\llbracket w \rrbracket_{\Gamma} - \mathbf{n}_{\gamma} \cdot \sigma_1 \cdot \llbracket \nabla \mathbf{u} \rrbracket_{\Gamma} \cdot \mathbf{n}_{\gamma}) \delta a \, dS. \quad (32)$$

Variations with respect to displacement. For given Γ , the potential energy is those of a two-phase linear composite, then for an equilibrium state, the energy is minimum among the set of admissible displacements:

$$\mathbf{u} \in K.A = \{ \mathbf{u}^* / \llbracket \mathbf{u}^* \rrbracket_{\Gamma} = 0, \quad \mathbf{u}^* = \mathbf{u}^d \text{ over } \partial\Omega_u \}. \quad (33)$$

The solution \mathbf{u} for this minimum satisfies $\frac{\partial \mathcal{E}}{\partial \mathbf{u}} \delta \mathbf{u} = 0$, which is exactly:

$$\begin{aligned} 2\varepsilon(\mathbf{u}) &= \nabla \mathbf{u} + \nabla^t \mathbf{u}, \quad \sigma_i = \frac{\partial w_i}{\partial \varepsilon} = \mathbb{C}_i : \varepsilon(\mathbf{u}), \quad \operatorname{div} \sigma_i = 0, \text{ over } \Omega_i, \\ \llbracket \sigma \rrbracket_{\Gamma} \cdot \mathbf{n}_{\gamma} &= 0, \text{ over } \Gamma, \quad \mathbf{n} \cdot \sigma = \mathbf{T}^d, \text{ over } \partial\Omega_T. \end{aligned} \quad (34)$$

Hill's orthogonality conditions.. As $\llbracket \mathbf{u} \rrbracket_{\Gamma} = 0$, a vector $U(s)$ exists such that $\llbracket \nabla \mathbf{u} \rrbracket_{\Gamma} = \mathbf{U} \otimes \mathbf{n}_{\gamma}$, then Hill's orthogonality conditions [27] are fulfilled:

$$\llbracket \sigma \rrbracket_{\Gamma} \cdot \mathbf{n}_{\gamma} = 0, \quad \llbracket \mathbf{u} \rrbracket_{\Gamma} = 0, \quad \llbracket \sigma \rrbracket_{\Gamma} : \llbracket \varepsilon \rrbracket_{\Gamma} = 0. \quad (35)$$

Variations with respect to Γ . The variations of the potential energy with respect to Γ are described by motion with normal velocity $\delta a(s)$:

$$\frac{\partial \mathcal{E}}{\partial \Gamma} \delta \Gamma = - \int_{\Gamma} G(s) \delta a(s) \, dS. \quad (36)$$

Using (32,35) the driving force associated to the Γ motion is obtained as the local energy release rate G :

$$G = \llbracket w \rrbracket_{\Gamma} - \sigma : \llbracket \varepsilon \rrbracket_{\Gamma}. \quad (37)$$

as proposed in [28, 29, 30, 31]. When interface is moving, the properties of sound material change to those of transformed material, and a dissipation can occur.

Dissipation and evolution of Γ . The total dissipation due to the motion of Γ is

$$D_m = \int_{\Gamma} G(s) a(s) \, dS. \quad (38)$$

The motion $a(s)$ can be defined by a kinetic relation given by a function $\phi(G)$ such that $a(s) = \frac{d\phi}{dG}$ ([28, 31]). Here, we consider non regular kinetic function. The motion is governed by a normality law based on the driving force G

$$s \in \Gamma, \quad a(s) \geq 0, \quad G(s) \leq G_c, \quad (G - G_c) a(s) = 0, \quad (39)$$

then $a(s)$ is defined on the set \mathcal{K}_{Γ}

$$\mathcal{K}_{\Gamma} = \{a^*(s), s \in \Gamma / a^*(s) \geq 0 \text{ if } G(s) = G_c, a^*(s) = 0 \text{ otherwise}\}. \quad (40)$$

In these framework, two families of models are now considered : models without or with dissipation.

Reversible behaviour. When there is no dissipation, whatever is the loading history, contribution over Γ vanishes, this is realized for two cases

- $G_c = \infty$, then $a = 0$, the surface Γ is always fixed. There is no transformation.
- $G_c = 0$, then $G = 0$ and a can be positive. Two situations are possible depending on the constant H .

- $H = 0$, a can be positive and the transformation is uncontrolled by the loading;
- $H > 0$, the change of energy between the two phases controls the transformation as in phase transformation occurring in memory alloy or in pseudo-elasticity, examples can be founded in [32, 33].

A model with dissipation. The critical value G_c is finite. The surface Γ is a moving surface whose velocity a is governed by the normality law. The surface is defined by the implicit equation

$$G(X_\Gamma, t) \leq G_c, \quad X_\Gamma \in \Gamma. \quad (41)$$

For this particular behaviour, the rate boundary value problem has been presented in [15, 29] and criterion of stability and of bifurcation of evolution problems have been proposed based on discussion of existence and uniqueness.

Remark. When the dissipated energy depends only on the actual state, we can introduce $\mathcal{W}_d = \int_{\Omega_1} G_c \, d\Omega$ and add this term to the potential energy

$$\mathcal{E}_d = \mathcal{E} + \mathcal{W}_d. \quad (42)$$

The problem of evolution is governed by

$$\frac{\partial \mathcal{E}_d}{\partial \Gamma}(\Gamma^* - \Gamma) = \int_{\Gamma} ([[w]]_\Gamma - \sigma : [[\varepsilon]]_\Gamma - G_c)(a - a^*) \, dS \geq 0, \forall a^* \in \mathcal{K}_\Gamma. \quad (43)$$

This point of view can be employed, but the separation between dissipated energy \mathcal{W}_d and stored energy $\int_{\Omega_1} H \, d\Omega$ must be specified.

3.4. Examples on a bar

A bar is decomposed into two domains, one $[0, \Gamma]$ with Young's modulus E_1 , and the complementary part $[\Gamma, L]$ made with sound material (E_0). The bar is loaded by applying displacement: $u(0) = 0$, $u(L) = \Delta L$, Δ is the global strain. The local stress $\sigma(x)$ is uniform. We discuss models without or with dissipation.

3.4.1. Reversible behaviour with $H > 0$

The stress is uniform, then the strain is piecewise uniform. Consider Δ the total strain, ε_0 the strain in initial phase with modulus E_0 , ε_1 the strain in the transformed phase, with modulus E_1 , $E_0 > E_1$. The proportion of transformed phase is denoted by z . The bar is a composite, where the two phases are separated by a boundary Γ with position zL . The total strain satisfies

$$\Delta = z\varepsilon_1 + (1 - z)\varepsilon_0. \quad (44)$$

The condition $0 \leq z \leq 1$ is taken into account by a Lagrange multiplier γ :

$$z(z - 1) \leq 0, \quad \gamma \geq 0, \quad \gamma z(z - 1) = 0. \quad (45)$$

The total strain is imposed by a Lagrange's multiplier γ_Δ associated to the relation (44). The potential energy of the bar is given by unit length ([32]):

$$\begin{aligned} \mathcal{E}(z, \varepsilon_0, \varepsilon_1, \gamma_\Delta, \gamma; \Delta) &= zw_1(\varepsilon_1) + (1 - z)w_0(\varepsilon_0) \\ &+ \gamma_\Delta(\Delta - z\varepsilon_1 - (1 - z)\varepsilon_0) + \gamma z(z - 1). \end{aligned} \quad (46)$$

This energy is stationary with respect to all unknowns $(z, \varepsilon_0, \varepsilon_1, \gamma, \gamma_\Delta)$

$$\begin{aligned} \frac{\partial \mathcal{E}}{\partial \gamma} \delta \gamma &= z(z - 1) \delta \gamma = 0, \quad \frac{\partial \mathcal{E}}{\partial \gamma_\Delta} \delta \gamma_\Delta = (\Delta - z\varepsilon_1 - (1 - z)\varepsilon_0) \delta \gamma_\Delta = 0, \\ \frac{\partial \mathcal{E}}{\partial \varepsilon_1} &= z(E_1 \varepsilon_1 - \gamma_\Delta) = 0, \quad \frac{\partial \mathcal{E}}{\partial \varepsilon_0} = (1 - z)(E_0 \varepsilon_0 - \gamma_\Delta) = 0, \\ G = -\frac{\partial \mathcal{E}}{\partial z} &= -\frac{1}{2} E_1 \varepsilon_1^2 - H + \frac{1}{2} E_0 \varepsilon_0^2 + \gamma_\Delta(\varepsilon_1 - \varepsilon_0) - \gamma(2z - 1) = 0. \end{aligned} \quad (47)$$

Taking account of (45): $\gamma \geq 0$ and $\delta \gamma \neq 0$ if and only if $z = 0$ or $z = 1$; otherwise $\gamma = 0$ and $\delta \gamma = 0$. This defines the potential value of z .

The reaction associated to Δ is given by

$$\frac{\partial \mathcal{E}}{\partial \Delta} = \gamma_\Delta = \Sigma. \quad (48)$$

The Lagrange's multiplier γ_Δ is the global stress.

Consider now an increasing strain Δ from initial stress free state, the response undergoes three main phases.

Phase I- $z = 0$. At the beginning only phase (0) exists, then $\gamma \geq 0$ and $G = 0$.

$$z = 0, \quad \frac{1}{2}E_1\varepsilon_1^2 + H + \frac{1}{2}\Sigma\varepsilon_0 - \Sigma\varepsilon_1 - \gamma = 0. \quad (49)$$

For $z = 0$, ε_1 is not determined, this phase does not exist yet. Hence γ must be positive for all ε_1 , the minimum value for ε_1 determines the minimum value for γ , then

$$E_1\varepsilon_1 = \Sigma, \quad \gamma = H + \frac{1}{2}\Sigma(\varepsilon_0 - \varepsilon_1) = H + \frac{1}{2}\Sigma^2\left(\frac{1}{E_0} - \frac{1}{E_1}\right) \geq 0. \quad (50)$$

The transformation begins when the stress Σ reaches critical value Σ_c defined by $\gamma = 0$.

Phase II-Transformation, $0 \leq z \leq 1$. When Δ is increasing from the state ($\Sigma = \Sigma_c$), the two phases coexist and $\gamma = 0$. The stress being uniform, we have

$$0 = \frac{1}{2}\Sigma(\varepsilon_0 - \varepsilon_1) + H = 0, \quad \Sigma = E_0\varepsilon_0 = E_1\varepsilon_1. \quad (51)$$

During the transformation we have

$$\frac{1}{2}\Sigma^2\left(\frac{1}{E_0} - \frac{1}{E_1}\right) + H = 0, \quad (52)$$

and therefore

$$\Sigma = \Sigma_c, \quad \Delta = \Sigma_c\left(\frac{z}{E_1} + \frac{1-z}{E_0}\right). \quad (53)$$

The last equation defines the state z : when Δ is increasing, z grows to one.

Phase III-Total transformation, $z = 1$. Now, the phase 0 has disappeared, $\gamma \geq 0$, the condition of no dissipation is now

$$0 = -\frac{1}{2}\Sigma\varepsilon_1^2 + H - \frac{1}{2}E_0\varepsilon_0^2 + \Sigma\varepsilon_0 + \gamma, \quad (54)$$

ε_0 is now not defined, $\gamma \geq 0$ implies

$$\gamma = -H + \frac{1}{2}\Sigma^2\left(\frac{1}{E_1} - \frac{1}{E_0}\right). \quad (55)$$

Then, the relation is true when $\Sigma > \Sigma_c$, and $\Delta = \frac{\Sigma}{E_1}$ so this is satisfied when Δ is increasing from the end of the previous state.

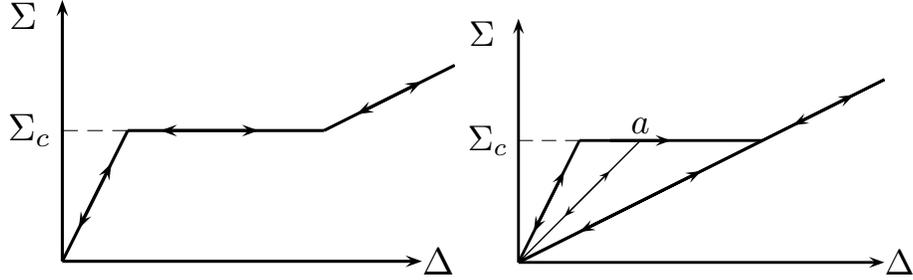


Figure 3: Reversible Phase transformation,(Left) ; with dissipation (Right) ; $\leftarrow - \rightarrow$ reversible path

Unloading path from the end of phase III. From such a final point, assume now that Δ is decreasing, then $\gamma \geq 0$ until Σ equal to Σ_c , at this stage $\gamma = 0$; from that state, the equations are those of step II, then the relations between $\Delta(z)$ is recovered, z is decreasing as Δ did, until $z = 0$. From that point, the relations of step one are recovered, until $\Delta = 0$. The response is plotted on Figure 3 (left). Some more general models corresponding to this framework can be found in [32, 33, 34, 35].

3.4.2. A model with dissipation : a quasi-brittle material

Assume $H = 0$ and consider now that Γ is a moving surface. As previously, the bar is loaded by applying displacement: ($\mathbf{u}(0) = 0$, $\mathbf{u}(L) = \Delta L$). The local stress σ is uniform with value Σ . Under increasing global strain Δ the response of the bar is decomposed in three phases.

Phase I- Elastic behaviour. The position Γ being known, the bar is an uni-axial composite with a a global stiffness defined by

$$\frac{1}{E^{hom}} = \frac{\Gamma}{LE_1} + \left(1 - \frac{\Gamma}{L}\right) \frac{1}{E_0}. \quad (56)$$

There is no propagation if

$$\frac{\Sigma^2}{2} \left(\frac{1}{E_1} - \frac{1}{E_0} \right) \leq G_c, \quad \Sigma \leq \Sigma_c, \quad (57)$$

with

$$\frac{\Sigma_c^2}{2} \left(\frac{1}{E_1} - \frac{1}{E_0} \right) = G_c. \quad (58)$$

Phase II- Propagation. When $G = G_c$, $\Sigma = \Sigma_c$ and the propagation is possible. With respect to the normality law, the interface is moving if and only if $\Sigma = \Sigma_c$, and the definition of the global strain imposed

$$\dot{\Delta} = \frac{a}{L} \left(\frac{1}{E_1} - \frac{1}{E_0} \right) \Sigma_c, \quad (59)$$

where a is the normal velocity of the moving surface. This relation is due to the continuity of the displacement at the interface Γ .

Phase III - Total transformation. When the bar is totally transformed, the material is now homogeneous with modulus E_1

Note the main differences between the two examples. For phase transformation, with no dissipation, paths for loading and unloading are always the same. For transformation with dissipation, the unloading path depends on the state of transformation and the modulus of elasticity is always decreasing with the irreversibility of the transformation, that is a damage model, (see figure 3).

4. Models with damage gradient

To avoid sharp interface, more regular description is proposed now. The damage is now continuous and the sharp interface is replaced by a continuous transition zone. In this zone, damage is continuous but its gradient is determined by additional relations. In the same spirit of gradient damage models are phase-field models. They are motivated from the elliptic regularization [36] of the Mumford-Shah functional used for image segmentation [37]. This point of view is generally used for initiation and propagation of cracks. We introduce in the same spirit a stored energy function of d and a quadratic terms on ∇d :

$$\psi(d, \nabla d) = H(d) + \frac{1}{2} g_c \|\nabla d\|^2. \quad (60)$$

Such descriptions have been used in [11, 12, 14, 20]

4.1. The total potential energy and its variations

Now, the potential energy has the value

$$\mathcal{E}(\mathbf{u}, d) = \int_{\Omega} w(\varepsilon, d) + \psi(d, \nabla d) \, d\Omega - \int_{\partial\Omega_{\Gamma}} \mathbf{T} \cdot \mathbf{u} \, dS. \quad (61)$$

Along Γ bonding is perfect, then displacements and stress vectors are continuous. We consider now that damage is continuous too, then the moduli of elasticity are continuous and hence the strain energy is also continuous.

Possible discontinuities are derived only from the energy ψ . Consider Γ a surface with normal vector \mathbf{n}_{γ} where ∇d is discontinuous. Then variations of potential energy with respect to \mathbf{u} are unchanged, and due to the compatibility on the discontinuity of ∇d we have

$$\begin{aligned} \frac{\partial \mathcal{E}}{\partial d} \delta d + \frac{\partial \mathcal{E}}{\partial \Gamma} \delta \Gamma = & - \int_{\Omega} Y^* \delta d \, d\Omega + \int_{\partial\Omega} g_c \nabla d \cdot \mathbf{n} \, \delta d \, dS + g_c \int_{\Gamma} \mathbf{n}_{\gamma} \cdot [[\nabla d]]_{\Gamma} \delta d_0 \, dS \\ & g_c \int_{\Gamma} (\mathbf{n}_{\gamma} \cdot \nabla d_d [[\nabla d]]_{\Gamma} \cdot \mathbf{n}_{\gamma} - \frac{1}{2} [[\|\nabla d\|^2]]_{\Gamma}) \delta a \, dS, \end{aligned}$$

with

$$Y^* = Y - h(d) + g_c \Delta d. \quad (62)$$

Using now the normality rule,

$$\dot{d} \geq 0, \quad Y^* - Y_c \leq 0, \quad (Y^* - Y_c) \dot{d} = 0. \quad (63)$$

The domain Ω is then decomposed into two sub-domains

- Ω^- where $Y^* - Y < 0$, then $\dot{d} = 0$,
- Ω^+ where $Y^* - Y = 0$, then $\dot{d} \geq 0$.

For a distribution of damage $d(x)$ over Ω , the decomposition (Ω^-, Ω^+) is known, and the variations $\delta d \geq 0$ are defined only on Ω^+ :

$$\dot{d} \in \mathcal{K}, \quad \delta d \in \mathcal{K} = \{ \dot{d}^* / \dot{d}^* \geq 0, \text{ over } \Omega^+, \dot{d} = 0, \text{ otherwise} \}. \quad (64)$$

This implies that

- discontinuities can appear only on the boundary $\partial\Omega^+$; if Γ is inside Ω^+ , $\delta d_0 \neq 0$, if $\Gamma \subset \partial\Omega^+ \cap \Omega^-$, $\delta d_0 = 0$,

- $\nabla d \cdot \mathbf{n} = 0$ on $\partial\Omega^+ \cap \partial\Omega$.

The last properties shows that $\nabla d \cdot \mathbf{n} = 0$ on $\partial\Omega$, this is true for the initial value. the evolution of d and ∇d are depending on the evolution of Ω^+ and on $\partial\Omega^+ \cap \partial\Omega$, $\delta d \neq 0$.

Then if there is a discontinuity an additional term along $\Gamma = \partial\Omega^+$ appears

$$G = g_c \left(\frac{1}{2} \llbracket \nabla d^2 \rrbracket_{\Gamma} - \mathbf{n}_{\gamma} \cdot \nabla d^+ \llbracket \nabla d \rrbracket_{\Gamma} \cdot \mathbf{n}_{\gamma} \right). \quad (65)$$

The total dissipation is then

$$D = \int_{\Omega} Y^* \dot{d} \, d\Omega + \int_{\Gamma} G \, a \, dS. \quad (66)$$

As for volume term, we adopt a normality rule for the evolution of Γ

$$s \in \Gamma, \quad a(s) \geq 0, \quad G \leq G_c, \quad a(s) (G - G_c) = 0. \quad (67)$$

A transition zone without surface dissipation.. We have several possibilities to have only volume dissipation.

- $G_c = \infty$ then $a = 0$, Γ is fixed, if G_c is inside Ω^+ , $\delta d \neq 0$ then $\nabla d \cdot \mathbf{n}_{\gamma}$ is continuous. the only possibility to have gradient discontinuity is on $\Gamma = \partial\Omega^+ \cap \Omega^-$.
- $G_c = 0$ then $G = 0$. For an iso- d , $\llbracket \nabla d \rrbracket_{\Gamma} = G \mathbf{n}_{\gamma}$ and $G = 0$ implies $\llbracket \nabla d \rrbracket_{\Gamma} \cdot \mathbf{n}_{\gamma} = 0$, that is the continuity of ∇d .

In the first case, the damage zone seems to be fixed, then the damage zone does not evolved ; then to ensure an evolution the best choice is to consider that $\llbracket \nabla d \rrbracket_{\Gamma} = 0$.

4.2. On the bar in extension

On a uni-axial bar, consider a continuous transition zone, of thickness l . The bar is fixed in $x = 0$ the displacement is imposed at extremal point $x = L$. Along the bar, the state of stress is uniform. The evolution of damage is given by the normality law

$$\dot{d} \geq 0, \quad Y^* - Y_c \leq 0, \quad (Y^* - Y_c) - h \dot{d} = 0. \quad (68)$$

The uniform solution is always possible during the phase of loading until the maximum value is reached see Fig.1. But from this point another solution is proposed. The bar is decomposed into two domains $\Omega^+ = [0, x_m], \Omega^- = [x_m, L]$ As dissipation occurs only inside the volume, the respect to normality law gives the damage distribution:

$$\frac{\Sigma^2}{2E\omega(d)} - Y_c d - H(d) + \frac{1}{2}g_c\left(\frac{dd}{dx}\right)^2 = Cst, \text{ over } \Omega^+. \quad (69)$$

The constant Cst is defined by the boundary condition in $d_m = d(0), d(x_m) = 0$

$$\frac{\Sigma^2}{2E\omega(d_m)} - Y_c d_m - H(d_m) = \frac{\Sigma^2}{2E}. \quad (70)$$

Then $\Sigma(d_m)$ is determined, integration of (68) gives the profile $d(x)$. Such a profile is given on figure 7, for the curve where $x_a = x_b$. When d_m tends to 0, the respect to the normality rule defines a critical value Σ_c for which appears a damaged zone. This can be considered as the critical value for the initiation of a defect.

This shows a possible bifurcation from the equilibrium path associated to the homogeneous solution. When $d(0) = 1$ the bar is broken, this gives a condition on the critical loading for an apparition of rupture. Initiation of defect can also be defined at the critical value for bifurcation point along the equilibrium path.

5. A model of graded damage

This model is based on convex analysis and an internal constraint is imposed such that the damage gradient is finite. The damage variable is submitted to two internal constraints.

- To take into account of $0 \leq d \leq 1$ a convex constraint can be introduced

$$\phi_1(d) = d(d - 1) \leq 0. \quad (71)$$

- In the case of graded damage materials [16, 17] a second convex constraint is imposed to control the gradient

$$\phi_2(d, \nabla d) = \|\nabla d\| - f(d) \leq 0. \quad (72)$$

this function is convex if f is concave, with $f(d) > 0$.

These convex constraints are imposed by introduction of Lagrange's multipliers γ_i or by indicators functions, these formulations are equivalent.

$$\gamma_i \geq 0, \quad \phi_i \leq 0, \quad \gamma_i \phi_i = 0. \quad (73)$$

5.1. The generalized model

In such description the generalized model has a local augmented free energy

$$\mathbb{L}(\varepsilon, d, \nabla d, \gamma_i) = w(\varepsilon, d) + H(d) + \gamma_1 \phi_1(d) + \gamma_2 \phi_2(d, \nabla d), \quad (74)$$

and we define the local state equations

$$\sigma = \frac{\partial w}{\partial \varepsilon}, \quad \mathbb{Y} = -\frac{\partial w}{\partial d}. \quad (75)$$

5.2. The equilibrium problem

Consider a body Ω . The external boundary is submitted to the boundary condition (BC. 3.3). The unknowns of the equilibrium problem of body Ω are displacement \mathbf{u} , damage d , the domain of sound material with boundary Γ .

5.3. On the regularity of the fields

Inside Ω , the displacement is continuous, but the other mechanical fields can be discontinuous. The bonding is perfect, then the displacement is continuous as well as the stress vector, and we assume that damage is continuous too. As damage is continuous, the moduli $\mathbb{C}(d)$ are continuous, the strain energy and $\nabla \mathbf{u}$ are continuous anywhere, but ∇d can be discontinuous.

5.4. The total potential energy

The total potential energy is given by

$$\mathcal{E}(\mathbf{u}, d, \gamma_i) = \int_{\Omega} \mathbb{L}(\varepsilon(\mathbf{u}), d, \nabla d, \gamma_i) \, d\Omega - \int_{\partial\Omega_T} \mathbb{T}^d \cdot \mathbf{u} \, dS. \quad (76)$$

Due to continuity conditions of the fields, it is obvious that the strain energy is continuous, $[[w]]_\Gamma = 0$. The variations of the potential energy are given in terms of $\delta \mathbf{u}$, δd , δa , $\delta \gamma_i$, then

$$\begin{aligned} \delta \mathcal{E} = & \int_{\Omega} (\sigma : \varepsilon(\delta \mathbf{u}) - \mathbf{Y} \delta d) \, d\Omega - \int_{bdVt} \mathbf{T}^d \cdot \delta \mathbf{u} \, dS + \int_{\Omega} \gamma_1 (2d - 1) \delta d \, d\Omega \\ & + \int_{\Omega} \gamma_2 \left(\frac{\nabla d \cdot \nabla \delta d}{\|\nabla d\|} - f' \delta d \right) \, d\Omega + \int_{\Omega} \phi_1 \delta \gamma_1 + \phi_2 \delta \gamma_2 \, d\Omega. \end{aligned} \quad (77)$$

After integration by parts we obtain ($\delta \mathbf{u} = 0$, over $\partial \Omega_u$):

$$\begin{aligned} \delta \mathcal{E} = & - \int_{\Omega} \operatorname{div} \sigma \cdot \delta \mathbf{u} \, d\Omega + \int_{\partial \Omega_T} (\mathbf{n} \cdot \sigma - \mathbf{T}^d) \cdot \delta \mathbf{u} \, dS + \int_{\Omega} \phi_1 \delta \gamma_1 + \phi_2 \delta \gamma_2 \, d\Omega \\ & - \int_{\Omega} \mathbf{Y}^* \delta d \, d\Omega + \int_{\Gamma} [[y_\Gamma^* \delta d]]_\Gamma \, dS + \int_{\partial \Omega} y^* \delta d \, dS. \end{aligned} \quad (78)$$

Variations with respect to displacement. For a given distribution of d , the system is in equilibrium, this implies that

$$\sigma = \frac{\partial w}{\partial \varepsilon}, \operatorname{div} \sigma = 0 \text{ in } \Omega, \mathbf{n} \cdot \sigma = \mathbf{T}^d, \text{ over } \partial \Omega_T. \quad (79)$$

Variations with respect to multipliers. The variations with respect to γ_1 and γ_2 define a partition of Ω : $\Omega = \Omega^- \cup \Omega_2^- \cup \Omega_2^+$:

$$\begin{cases} x \in \Omega^-, & \phi_1 = 0, \gamma_1 \geq 0, & \phi_2 \leq 0, \gamma_2 = 0, \\ x \in \Omega^+, & \phi_1 < 0, \gamma_1 = 0, & \begin{cases} x \in \Omega_2^-, & \phi_2 < 0, \gamma_2 = 0, \\ x \in \Omega_2^+, & \phi_2 = 0, \gamma_2 \geq 0. \end{cases} \end{cases} \quad (80)$$

5.4.1. Variations with respect to d and to Γ

We obtain three contributions

$$\int_{\Omega} -\mathbf{Y}^* \delta d \, d\Omega + \int_{\Gamma} [[y^* \delta d]]_\Gamma \, dS + \int_{\partial \Omega} y^* \delta d \, dS. \quad (81)$$

Along the surface Γ , damage is continuous, then

$$[[\delta d]]_\Gamma + \delta a [[\nabla d]]_\Gamma \cdot \mathbf{n}_\gamma = 0. \quad (82)$$

Consider now each term:

- Inside the volume : the definition of the driving force Y^* is obtained and due to the normality law we have:

$$x \in \Omega, \quad Y^* = Y - h + \nabla(\gamma_2 \nabla d) \frac{1}{f} - \gamma_1(2d - 1) \leq Y_c. \quad (83)$$

On Ω^+ , the variations must be compatible with the normality rule. The damage can evolve only on Ω^+ ,

$$\dot{d} \in \mathcal{K}, \delta d \in \mathcal{K}. \quad (84)$$

Then on Ω^+ , $\gamma_1 = 0$.

- Along Γ , using (82) we have $[[y^* \delta d]]_{\Gamma} = [[y^*]]_{\Gamma} \delta d^- - G \delta a$,

$$x \in \Gamma, \quad y^* = \gamma_2 \mathbf{n}_{\gamma} \cdot \frac{\nabla d}{\|\nabla d\|}, \quad G = \gamma_2^+ \mathbf{n}_{\gamma} \cdot \frac{\nabla d}{\|\nabla d\|} + [[\nabla d]]_{\Gamma} \cdot \mathbf{n}_{\gamma}. \quad (85)$$

- Along $\partial\Omega$, $y^* = \mathbf{n} \cdot \gamma_2 \frac{\nabla d}{\|\nabla d\|}$.

Study of possible discontinuities. Over Ω^- , we have $\gamma_2 = 0$. If $\Gamma \subset \Omega^+$ then $\delta d \geq 0$ and

- $\Gamma \subset \Omega_2^-$, then $y^* = 0$ because $\gamma_2 = 0$.
- $\Gamma \subset \Omega_2^+$, $\gamma_2^+ \geq 0$, $\gamma_2^- \geq 0$; $[[d]]_{\Gamma} = 0$ then $[[\phi_2]]_{\Gamma} = 0$, consequently $[[\|\nabla d\|]]_{\Gamma} = 0$.

The point x belongs to an iso-damage curve ; at that point, the normal vector to this level-set is \mathbf{n}_{γ} . Then $\nabla d^+ = \pm f(d) \mathbf{n}_{\gamma}$, $\nabla d^- = \pm f(d) \mathbf{n}_{\gamma}$. As $\Gamma \subset \Omega_2^+$, $\delta d^- \geq 0$, as $[[\|\nabla d\|]]_{\Gamma} = 0$, and consequently we have:

$$\begin{aligned} - & [[\gamma_2 \nabla d]]_{\Gamma} \cdot \mathbf{n}_{\gamma} = 0, \quad (\nabla d^+ - \nabla d) \cdot \mathbf{n}_{\gamma} = 0 \text{ then } \gamma_2^+ = \gamma_2^-, \\ - & [[\gamma_2 \nabla d]]_{\Gamma} \cdot \mathbf{n}_{\gamma} = 0 \text{ with } (\nabla d^+ + \nabla d^-) \cdot \mathbf{n}_{\gamma} = 0 \text{ then } \gamma_2^+ = \gamma_2^- = 0. \end{aligned}$$

The last possibility is when $\Gamma \subset \partial\Omega^+ \cap \Omega^-$. In this case $\gamma_2^- = 0$, the contribution on Γ is reduced to $G \delta a$ or equivalently $y_+^* \delta d^+$.

Then, some additional terms must be added to define the dissipation and the evolution of the boundary Γ . This can be made by introducing a normality law (67), then $a(s), \delta a(s)$ are fields belonging to the set \mathcal{K}_{Γ} .

The model of graded damage. For the model of graded damage, we have no contribution on Γ , the dissipation occurs on the volume only. This implies that $\gamma_2^+ = 0$ along Γ .

On external boundary. On the external boundary, we have $\gamma_2 \nabla d \cdot \mathbf{n} = 0$,

$$x \in \partial\Omega, \quad \begin{cases} \phi_2 < 0 & \gamma_2 = 0, \\ \phi_2 = 0 & \gamma_2 \geq 0. \end{cases} \quad (86)$$

When $\phi_2 = 0$ then $\|\nabla d\| > 0$, the condition $\gamma_2 \nabla d \cdot \mathbf{n}$ does not imply $\nabla d \cdot \mathbf{n} = 0$, but $\gamma_2 = 0$. This condition is one of the main difference with models of section 4.

5.5. The bar under uni-axial extension

We study now the bar with this new constitutive law. Assuming that a

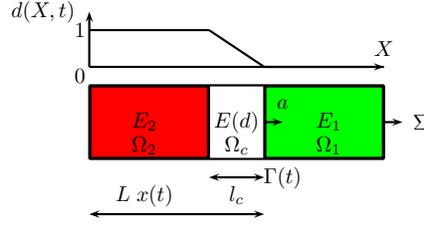


Figure 4: A model of continuous transition; profile of damage along a layer of finite thickness.

damaged zone is established from 0 to $x_m = \Gamma - l$, the common boundary with the sound material is on $x_m = \Gamma$. Then the Young modulus is a decreasing function of x , $E(x_o) = E_1, E(\Gamma) = E_0$. As the Young modulus depends on $d(\Gamma(t) - x)$, then

$$\dot{d} + a \nabla d \cdot \mathbf{e}_x = 0. \quad (87)$$

The dissipation is given as

$$D_m = a \int_{l_c} \frac{1}{2} \Sigma^2 \left(-\frac{E'_{,d}}{E^2} \right) d'_{,x} dx = a \Sigma^2 \int_1^0 \left(-\frac{E'_{,d}}{2E^2} \right) dd = \llbracket w \rrbracket_{\Gamma} a. \quad (88)$$

The dissipation does not depend on the profile $d(\Gamma - x)$. This is due to the absence of curvature of the front and to the hypothesis of local steady state. Consider now that the damage initiates at $x = 0$, the damage propagates inside

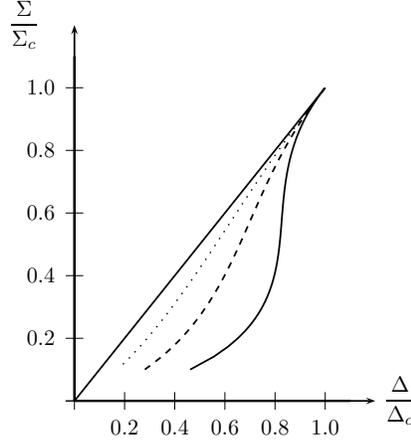


Figure 5: The bar in extension : $\omega = 1 - d, h = 0$, depending on L : $L = l_c$, " - "; $L = 2l_c$, " - - "; $L = 3l_c$, " . . "

the bar and its value at $x = 0$ becomes $d(0) = d_m$ at a moment.

Consider $\phi_2 = 0$ with $f(d) = \frac{1}{l_c}$, damage profile is

$$d(x) = d_m - \frac{x}{l_c}, \quad \Omega_2 = [0, x_m = l_c d_m]. \quad (89)$$

The Lagrange multiplier γ_2 satisfies the normality law

$$Y - Y_c - h(d) - \frac{1}{l_c} \frac{d\gamma_2}{dx} = 0. \quad (90)$$

Taking account of the relation $x = l_c(d_m - d)$, by integration of this equality with respect to d one obtain:

$$\frac{\Sigma^2}{2E\omega(d)} - Y_c d - H(d) - \frac{1}{l_c^2} \gamma_2 = Cst, \quad (91)$$

where the constant is determined by the boundary conditions $d(0) = d_m$, $d(x_m) = 0$ and $\gamma_2(0) = \gamma_2(x_m) = 0$. This defines the tension Σ compatible

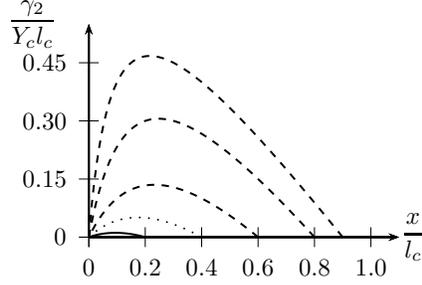


Figure 6: The Lagrange's multiplier γ_2 is increasing with increasing values of $d(0) = d_m = x_m/l_c : .2, .4, .6, .8, .9$

with the damage profile:

$$\frac{\Sigma^2}{2E} \left(\frac{1}{\omega(d_m)} - 1 \right) = Y_c(d_m) - H(d_m). \quad (92)$$

and also the value of the Lagrange's multiplier γ_2 , For $\omega = 1 - d, h(d) = 0$, we obtain

$$\gamma_2 = Y_c l_c^2 \frac{d(d_m - d)}{1 - d} \geq 0. \quad (93)$$

see figure 6. By integration of the constitutive law,

$$\varepsilon = \frac{\Sigma(d_m)}{\omega(d)}, \quad L\Delta = \int_0^L \varepsilon(x) dx, \quad (94)$$

we obtain the global response of the bar: $(\Sigma(d_m), \Delta(d_m))$. The corresponding curves are presented on figure 5, for different length $L = l_c, 2l_c, 3l_c$.

For the same functions $\omega(d), H(d)$ and the same values of d_m , the obtained profiles of damage, for the modelling with the damage gradient or the graded damage, are distinct, the global responses too. (See later comment on figure 7 at the end of Sec. 6).

6. A regularized graded damage model

For practical application it can be useful to regularized the graded damage model. It can be done by addition of a quadratic term $\|\nabla d\|^2$ as previously

or by using a Moreau-Yosida approximation of the convex constraint ϕ_2 on the form:

$$I_C = \frac{1}{2\eta} |\phi_2|_+^2. \quad (95)$$

Addition of a functional $\psi(d, \nabla d) = H(d) + \frac{c}{2} (||\nabla d||)^2$ can be used also and a discussion on the possible discontinuity on the damage gradient must be investigated. The reasoning is exactly the same as previously.

We consider that the dissipation occurs only in the volume, then ∇d has no discontinuity, this is a regularization of graded damage model. For this simple example, the problem of the bar is revisited.

6.1. On the bar in extension

We reconsider a one-dimensional bar of length L subject to an increasing elongation. The free energy density is now

$$w^c = \frac{1}{2}(1-d)E_o\varepsilon^2 + \frac{1}{2}c||\nabla d||^2, \quad (96)$$

where $c > 0$ is a parameter of regularization. The constraint $\phi_2 \leq$ is chosen as:

$$\phi_2(d) = ||\nabla d|| - \frac{1}{l_c} \leq 0. \quad (97)$$

The variation of the potential energy with respect to d implies that the driving force associated to d is now

$$Y^* = \frac{\Sigma^2}{2E_o(1-d)^2} - \frac{1}{l_c} \frac{d\gamma_2}{dx} + c\Delta d. \quad (98)$$

with the boundary condition:

$$\nabla d \cdot \mathbf{n} = 0, \text{ over } \partial\Omega. \quad (99)$$

We obtain two families of solutions. The first one is homogeneous solution, whereas the second gives initiation and growth of a defect. We consider the second family with initiation of a defect at $x = 0$. During damage evolution, two phases are distinguished, first during which $\phi_2 < 0$ and $\gamma_2 = 0$, a second phase during which the constraint is satisfied, and the regularization term as no contribution.

Actually condition $Y^* = Y_c$ with $\gamma_2 = 0$ allows us to obtain the damage distribution along the bar, by integration

$$\frac{\Sigma^2}{2E_o(1-d)} - Y_c d + \frac{1}{2}c||\nabla d||^2 = Cst. \quad (100)$$

The boundary conditions $\nabla d(0) \cdot \mathbf{n} = 0, \nabla d(L) \cdot \mathbf{n} = 0, d(L) = 0$ determine the constant as $Cst = \Sigma/2E_o$ assuming $d(0) = d_m$, the value of the stress is given by

$$\Sigma^2 = 2E_o Y_c (1 - d_m) = \Sigma_c^2 (1 - d_m). \quad (101)$$

This solution is valid until $\phi_2 < 0$, to obtain a value for which this condition is violated it is necessary that

$$K = \frac{c}{2l_c^2 Y_c} < 1 \quad (102)$$

Under this condition, a domain $[x_a, x_b]$ where $\phi_2 = 0$ appears and

$$d = d(x_a) + \frac{x_b - x}{l_c}, \quad x \in [x_a, x_b], \quad (103)$$

and γ_2 satisfies the conditions:

- For $x \in [x_a, x_b]$,

$$\begin{aligned} \gamma_2 &\geq 0, \quad \gamma_2(x_a) = \gamma_2(x_b) = 0, \\ Cst &= \frac{\Sigma^2}{2E(1-d)} - \frac{1}{l_c} \gamma_2 + \frac{c}{2l_c^2} - Y_c d, \end{aligned} \quad (104)$$

- $\Gamma \in \{x_a, x_b\}$

$$[[\nabla d]]_{\Gamma} = 0, \Gamma \in \{x_a, x_b\}, \quad \nabla d(0) = 0. \quad (105)$$

Finally we obtain $K = d(x_a)d(x_b)$ and $x^+ = x_a, x^- = x_b$

$$d(x^\pm) = \frac{1}{2}(d_m + K)(1 \pm \sqrt{1 - \frac{4K}{(d_m + K)^2}}). \quad (106)$$

For a given K the first value of damage d_o for which $\phi_2 = 0$ is fulfilled at the point $x_a = x_b$ is given by

$$d_o = 2\sqrt{K} - K. \quad (107)$$

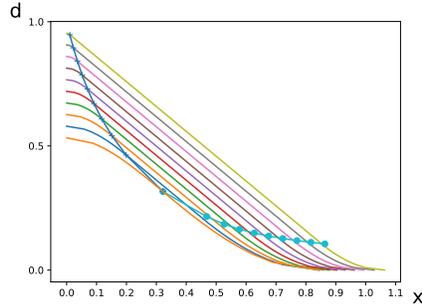


Figure 7: The damage profile $(x, d(x))$ for different $d(0) = d_m$, $(x_a, d(x_a)) : "$ +", $(x_b, d(x_b)) : "$ o"

The smaller is K , the more localized is damage near $x = 0$ during the first phase. The global response is depending of the length of the bar, and the profile of damage depends on the K value. We recognise on figure 7 the progression of damage inside the bar, for increasing value of d_m from d_o . The profile is linear with slope $1/l_c$ on segment $[x_a(d_m), x_b(d_m)]$.

On figure 7, when $x_a = x_b$ the damage profile corresponds to the response without ϕ_2 . This indicates that the damage profiles are identical for the same laws (70) $\omega(d), H(d), Y_c$ until $\phi_2(d, \nabla d) = 0$.

7. On the role of the curvature: example on a sphere

The role of the curvature of the front of damage is investigated, solving the evolution problem of sharp interface and graded damage for a sphere under radial loading.

7.1. The inhomogeneous sphere under radial loading

Consider a sphere with external radius R_e composed by elastic linear materials with same shear modulus μ_o and bulk modulus $K(r)$ depending on radius r . Under radial loading the displacement is $\mathbf{u} = u(r)\mathbf{e}_r$, the strain becomes

$$\varepsilon = \frac{du}{dr} \mathbf{e}_r \otimes \mathbf{e}_r + \frac{u}{r} (\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\phi \otimes \mathbf{e}_\phi), \quad (108)$$

the stress is reduced to

$$\boldsymbol{\sigma} = \sigma_{rr} \mathbf{e}_r \otimes \mathbf{e}_r + \sigma_{\theta\theta} \mathbf{e}_\theta \otimes \mathbf{e}_\theta + \sigma_{\phi\phi} \mathbf{e}_\phi \otimes \mathbf{e}_\phi, \quad (109)$$

where $\sigma_{\theta\theta} = \sigma_{\phi\phi}$. Using the local constitutive law, the displacement \mathbf{u} satisfies the conservation law of momentum

$$-\frac{d}{dr} \left(\Lambda(r) \left(\frac{du}{dr} + 2\frac{u}{r} \right) \right) = 0, \quad (110)$$

where $\Lambda(r) = \lambda(r) + 2\mu_o$; λ, μ are the Lamé's moduli of elasticity. $3\Lambda(r) = 3K(r) + 4\mu_o$. At the center of the sphere ($r = 0$) the displacement vanishes, then the solution is

$$r^2 u(r) = A I(r), \quad I(r) = \int_0^r \frac{t^2}{\Lambda(t)} dt. \quad (111)$$

A is determined by the boundary condition at surface ($r = R_e$):

$$u(R_e) = \Delta R_e, \quad R_e^3 \Delta = A I(R_e). \quad (112)$$

The total strain energy of the sphere is given by

$$\mathcal{E} = 2\pi \int_0^{R_e} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} r^2 dr = \frac{1}{2} \int_{r=R_e} \boldsymbol{\sigma}(R_e) \cdot \mathbf{u}(R_e) dS = \pi R_e^2 \sigma_{rr}(R_e) u(R_e). \quad (113)$$

As the radial stress (σ_{rr}) is

$$\sigma_{rr} = \lambda \left(\frac{du}{dr} + 2\frac{u}{r} \right) + 2\mu_o \frac{du}{dr} = A - 4\mu_o \frac{u}{r}, \quad (114)$$

the value of the total strain energy becomes

$$\mathcal{E} = 4\pi R_e^3 \Delta^2 \left(\frac{R_e^3}{I(R_e)} - 2\mu_o \right). \quad (115)$$

At point $r = R_e$, $\sigma_{rr}(R_e) = A - 4\mu_o \Delta = \Sigma$. The above equations are valid for any distribution of the elastic modulus $\Lambda(r)$. We consider now two examples, one with a sharp interface, another for graded damage modelling.

7.2. The sharp interface

For a sharp interface, the sphere is composed with two elastic materials with properties $\Lambda_o = \lambda_o + 2\mu_o$, $\Lambda_1 = \lambda_1 + 2\mu_o$. Then the integral I depends on the position of the interface Γ between the two materials

$$J(\Gamma) = I = \int_0^\Gamma \frac{t^2}{\Lambda_1} dt + \int_\Gamma^{R_e} \frac{t^2}{\Lambda_o} dt. \quad (116)$$

The volume fraction c of phase 1 is $c = (\Gamma/R_e)^3$. The boundary condition implies that

$$4\mu_o\Delta = A(3K_o c_o + 4\mu_o). \quad (117)$$

When $K_1 = 0$, the solution is solution for a cavity, because we have $\sigma_{rr}(\Gamma) = 0$ in this case. We consider now this case.

The energy release rate. When the interface is moving, with velocity $a = \dot{\Gamma}$, the total strain energy changes when Δ is fixed. Then the dissipation is

$$D_m = -\frac{\partial \mathcal{E}}{\partial \Gamma} \dot{\Gamma} = 4\pi A^2 \frac{\partial J}{\partial \Gamma} a = 4\pi \Gamma^2 G \dot{\Gamma}. \quad (118)$$

The energy release rate associated to the interface motion is then

$$G(\Delta, \Gamma) = A^2 \frac{\Lambda_o - \Lambda_1}{\Lambda_o \Lambda_1}. \quad (119)$$

Evolution of the cavity. The evolution of Γ is governed by the normality law

$$a \geq 0, \quad G - G_c \leq 0, \quad a(G - G_c) = 0. \quad (120)$$

The inequality $G(\Delta, \Gamma) \leq G_c$ gives an implicit equation of the moving surface taking account of the definition of A .

The critical state. When $G = G_c$, $A = A_c$ and we define the critical strain \mathbf{E}_c and a critical stress Σ_c

$$A_c^2 = G_c \frac{\Lambda_o \Lambda_1}{\Lambda_o - \Lambda_1}, \quad 9\Delta_c = \frac{G_c}{\Lambda_o - \Lambda_1} \frac{\Lambda_1}{\Lambda_o}, \quad \Sigma_c = \sigma_{rr}(R_e) = 3K_o(1 - c)A_c. \quad (121)$$

The evolution of the composite sphere. The initial value Γ is given. Consider the global strain Δ is increasing. The global response is those of a composite sphere with linear elastic behaviour, until the Δ_c value is reached.

From that state, if the radial expansion Δ is imposed, the interface moves, and the global response is

$$\Delta(\Gamma) = \frac{A_c}{4\mu_o} (3K_o c(\Gamma) + 4\mu_o) \quad \Sigma = \sigma_{rr}(R_e) = 3K_o A_c (1 - c(\Gamma)). \quad (122)$$

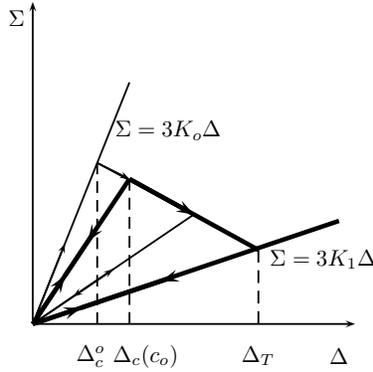


Figure 8: The sharp interface : the global response

This value is valid until $\Gamma = R_e$. The material is totally broken.

The response is obtained also for $0 < K_1 < K_o$ for which the energy release rate is

$$G = 9L^2(K_o - K_1)(3K_1 + 6\mu_o)(3K_o + 4\mu_o), \quad (123)$$

$$L = \frac{\Delta}{3K_1 + 4\mu_o + 3c(K_o - K_1)}.$$

Initiation of a defect. On figure 8, the value Δ_c^o is the value of $\Delta_c(\Gamma)$ when the radius Γ vanishes. This is the critical value of evolution for an infinitesimal spherical defect.

This point can be viewed as a bifurcation point, or an analysis of imperfection for the problem of evolution of a homogeneous sphere with compressibility K_o and the evolution of a perturbed system by a vanishing spherical defect. This analysis of bifurcation gives a condition of initiation of defect which depends on the geometry of the imperfection [8].

7.3. Case of a cavity

The case of a cavity is obtained with $K_1 = 0$. The evolution of the radial stress $\sigma_{rr}(r)$ is shown on figure 9. We see the propagation of damage regarding the value $R, \sigma_{rr}(R) = 0$ as function of Δ .

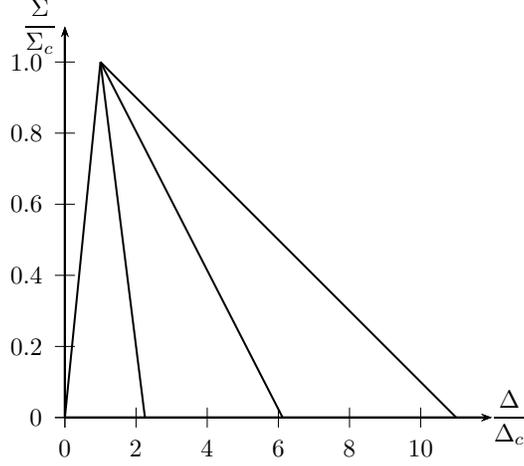


Figure 9: The sharp interface for a cavity : $\sigma_{rr}(R)$, for $R/R_e = .2, .4, 1$, $R_i/R_e = .1$

7.4. A graded damaged sphere

Consider now the graded damage behaviour. For a given distribution $d(r)$, $\nabla d = d'(r)\mathbf{e}_r$, $\|\nabla d\| = 1/l_c$, $d(r) = d(a) \pm (r - a)/l_c$. We consider particular evolution of the elastic modulus $\Lambda(d)$.

$$\frac{1}{\Lambda} = \frac{1-d}{\Lambda_o} + \frac{d}{\Lambda_1}, \quad (124)$$

The integrals $I(r)$ are now depending on the definition of d and on the local distribution $\Lambda(r)$ which evolves with the position of the interface Γ .

Under increasing loading, after a critical value, a damaged zone appears and develops until a finite thickness l_c is reached. After this phase of elaboration, the damage zone propagates as a layer with constant thickness l_c . This point of view implies that d varies from 0 to 1 on the distance l_c . Under the radial loading, we consider that d depends on r and $d(r) = \frac{\Gamma - r}{l_c}$.

Formation of a transition zone. During the formation of the transition zone, $\Gamma \leq l_c$ and the damage parameter takes the values:

$$\begin{cases} r \leq \Gamma, & d(r) = \frac{\Gamma - r}{l_c}, \\ r \geq \Gamma, & d(r) = 0. \end{cases} \quad (125)$$

Propagation of the transition zone. When the transition zone has a thickness equal to l_c , $\Gamma \geq l_c$ and the damage parameter satisfies:

$$\begin{cases} 0 \leq r \leq \Gamma - l_c, & d = 1, \\ \Gamma - l_c \leq r \leq \Gamma, & d = \frac{\Gamma - r}{l_c}, \\ \Gamma \leq r \leq R_e, & d = 0. \end{cases} \quad (126)$$

With these definitions, we can study the initiation of a small defect in an homogeneous sphere.

The total dissipation.. The total dissipation is reduced to the volume term $\int_{\Omega} Y \dot{d} \, d\Omega$, where $Y = -\frac{\partial w}{\partial d}$ is the local energy release rate:

$$Y = -\frac{1}{2} t r^2(\varepsilon) \frac{\partial \Lambda}{\partial d} = -\frac{A^2}{2\Lambda^2(d)} \frac{d\Lambda}{dd} \leq Y_c, \quad (127)$$

and

$$D_m = \int_{\Omega} Y \dot{d} \, d\Omega = -2\pi A^2 \int_0^{R_e} \frac{1}{2\Lambda^2 l_c} \frac{d\Lambda}{dd} r^2 \, dr \, \dot{\Gamma}_o, \quad (128)$$

which is nothing that:

$$D_m = 2\pi A^2 \frac{d}{d\Gamma} \left(\int_0^{R_e} \frac{\rho^2}{\Lambda(d)} \, d\rho \right) \dot{\Gamma}_o \leq 2\pi Y_c \int_o^{R_e} \frac{\rho^2}{l_c} \, d\rho \dot{\Gamma}, \quad (129)$$

taking account of the relation between d and Γ .

The equilibrium solution is given by

$$r^2 u(r) = A \int_0^r \frac{\rho^2}{\Lambda(\rho)} \, d\rho = A I(r). \quad (130)$$

We study now, the evolution of the damage during an increasing loading Δ .

Phase I. Initiation of the transition zone $\Gamma \leq l_c$.

$$J(\Gamma) = \int_0^{\Gamma} \left(\frac{d(\rho)}{\Lambda_1} + \frac{1 - d(\rho)}{\Lambda_o} \right) \rho^2 \, d\rho + \int_{\Gamma}^{R_e} \frac{\rho^2}{\Lambda_o} \, d\rho = \frac{R_e^3}{3\Lambda_o} + \frac{\Lambda_o - \Lambda_1}{\Lambda_o \Lambda_1} \frac{\Gamma^4}{12l_c}.$$

The boundary condition imposes that $R_e^3 \Delta = A J(\Gamma)$. The dissipation gives the definition of the equivalent energy release rate G

$$G = A^2 \frac{\partial J}{\partial \Gamma} = A^2 \frac{\Lambda_o - \Lambda_1}{\Lambda_o \Lambda_1} \leq Y_c. \quad (131)$$

During this phase ($b \Lambda_1 \Lambda_o l_c = \Lambda_1 - \Lambda_o$), the displacement is

$$\begin{cases} r \leq \Gamma, & r^2 u = A \left(\left(\frac{1}{\Lambda_o} - b\Gamma \right) \frac{r^3}{3} + b \frac{r^4}{4} \right), \\ r \geq \Gamma, & 12r^2 u = A \left(\frac{4r^3}{\Lambda_o} - b\Gamma^4 \right), \end{cases} \quad (132)$$

and

$$R_e^3 \Delta = A \left(\frac{R_e^3}{3\Lambda_o} - \frac{b\Gamma^4}{12} \right), \quad \Sigma = A \left(\frac{K_o}{\Lambda_o} + b\mu_o \frac{\Gamma^4}{3R_e^3} \right) = A - 4\mu_o \Delta. \quad (133)$$

During the formation of the transition zone, the value of $A = A_c$ is constant, this gives the same value than the composite sphere with sharp interface at the limit $d(0) = 0^+$, but for the initiation of a kernel of damaged material with modulus Λ_1 , the damage parameter is $d = 1$. For this state, the strain critical value is determined when $\Gamma = l_c$ and we obtain Δ_c^1 :

$$\Sigma = A - 4\mu \Delta_c^1, \quad \Delta_c^1 = A \frac{J(l_c)}{R_e^3}. \quad (134)$$

This strain critical value is greater than the value for the composite sphere with the sharp interface because

$$J(l_c) = J(0^+) + \frac{\Lambda_o - \Lambda_1}{\Lambda_o \Lambda_1} \frac{l_c^3}{12}. \quad (135)$$

The value for the sharp interface is recovered with $l_c = 0$, this is natural, the moving layer being reduced to a sharp interface.

Here, the solution of homogeneous sphere gives a critical load for bifurcation at point $A(\Delta) = A_c$, then from this point a kernel of damaged material is initiated and a moving **layer** begins to propagate from the center. When the value of damage $d(0)$ at the center reaches **the value $d(0) = 1$ a cavity appears** and after grows. This describes initiation of a defect. The critical value for initiation of a defect obtained with ($Y(0) = Y_c$) or of a cavity $d(0) = 1$ are not the same, if the first one is local and depend only on mechanical characteristic, the second depends on the loading history. This has been discuss in [8].

8. Conclusion

The discussion of the regularity of damage parameter implies different modelling of damage evolution associated to different **concepts** of dissipation, with

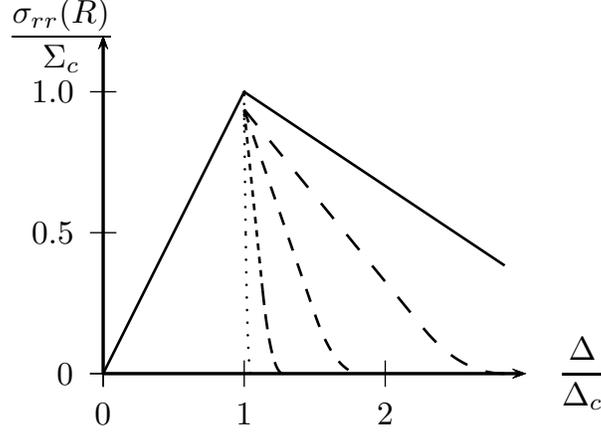


Figure 10: The local stress $\sigma_{rr}(r)$, $r/R_e \in \{.2, .3, .5, .7, .9, 1\}$

distinction between volume dissipation, and dissipation according to moving surface of mechanical discontinuities.

In this case, the propagation of the damage zone is described by the position of this interface and discontinuities of mechanical fields are present. To avoid such strong discontinuities, the model is related to a moving layer as in gradient damage modelling without discontinuities of damage. In this case, damage gradient can be discontinuous, and the damage gradient can be regularized by additional quadratic terms as in phase field, or by a convex constraint on his norm. The last description gives a physical parameter l_c which is directly connected to the thickness of the moving layer.

As well as the phase field, the graded damage model can be used to describe in the same framework initiation of defect and its propagation. Problem of stability and bifurcation of solution must be also investigated. In the model of uni-axial, after a maximum load, the solution loses its uniqueness, bifurcation occurs. In this case, additional complementary constraint on volume of the damaged zone is a potential way to control damage evolution.

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