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On a continuum theory for crack propagation in brittle materials

Fernando P. Duda[1)] and Angela C. Souza[2)]

1) Programa de Engenharia Mecânica, COPPE/UFRJ, Rio de Janeiro, RJ
2) Departamento de Engenharia Mecânica, LMTA/UFF, Niterói, RJ

ABSTRACT

This paper is concerned with the development of a theory for crack propagation in brittle solids. In order to characterize the cohesion state of the material, an order parameter field, which is related to the population of defects, is introduced. The microforce system, which acts in response to changes in the population of defects, is introduced and it is presumed consistent with its own balance, the microforce balance. Kinetic equations are obtained from the microforce balance and appropriate constitutive equations. The theory, which is described within the framework of modern continuum mechanics, can be considered as the first step toward a unifying route to incorporate not only physical processes on the microscale but also non-local effects.

INTRODUCTION

Recently, Aranson et al [1] presented a continuum field model for crack propagation in brittle amorphous solids. In addition to the displacement field $\mathbf{u}$, they introduced an order parameter α, which is related to the cohesion in the amorphous materials. In the context of linear isotropic viscoelasticity, the equations for the displacement were obtained from the standard force balance whereas the equation for the order parameter was obtained according to Landau ideas on phase transitions. Despite the success in describing important features of crack propagation such as crack initiation, propagation, dynamic fracture instability, crack branching, and fragmentation, the model proposed by Aranson et al is not thermodynamically consistent. In particular, it is not clear how the coupling between deformation and damage process is made.

This paper is concerned with the development of a mechanical framework to model crack propagation in brittle materials, under isothermal conditions. The framework to be developed is described within the scheme of modern continuum mechanics (see the introduction of Fried and Gurtin [2]). Following this scheme, we characterize the cohesion by the order paramenter α, which is related with the population of point defects (e.g. microcraks): it varies from 1 outside the crack (no defects) to 0 inside the crack (all the atomic bonds are broken). In addition to the standard force system, which is associated to $\mathbf{u}$ and acts in response to deformational changes, we introduce the microforce system, which acts in response to changes in the population of defects and it is associated to α. While the standard force system is presumed consistent with the force and moment balances, the microforce system is presumed consistent with its own balance, the microforce balance. To define a particular material, we introduce the constitutive equations, which are presumed to be consistent with the dissipation inequality.

The emphasis here is on determining those results which rely on features common to a wide class of behaviors rather than on specific and detailed features of any particular case. Primary among the results of this kind is the derivation of the evolution law for α in which criteria for the nucleation and growth of flaws and for definition of fracture based on attainment of some specified flaw population or density naturally emerge. Also, strain-rate effects are incorporated in the theory.

The paper is organized as follows: In Section 2 kinematics is developed. Then, we introduce, the basic laws in Section 3. We consider the constitutive equations in Section 4, where the constitutive assumptions are introduced and, by using the Coleman-Noll procedure, restrictions on the constitutive equations are obtained. In Section 5, as a consequence of the microforce balance, the kinetic equation is obtained.

We have adopted the notation commonly used in continuum mechanics [3]. Symbols and quantities are defined on the first time they appear in this paper.

KINEMATIC

We consider a homogeneous body $\mathcal{B}$, identified with the region of space it occupies in a fixed reference configuration. A motion maps the particle located at $\mathbf{x}$, in $\mathcal{B}$ at a time t, to a new location $\mathbf{y}$:

$$\mathbf{y}(\mathbf{x}, t) = \mathbf{x} + \mathbf{u}(\mathbf{x}, t), \tag{1}$$

where $\mathbf{u}$ is the displacement. The deformation gradient is denoted by $\mathbf{F}$:

$$\mathbf{F} = \mathbf{I} + \nabla \mathbf{u}, \tag{2}$$

where $\mathbf{I}$ is the identity tensor.

The local cohesion state of the material is described by a single scalar field $\alpha(\mathbf{x}, t)$ in $[0, 1]$, with gradient:

$$\mathbf{p} = \nabla \alpha. \tag{3}$$

BASIC LAWS

In this section we introduce the basic laws of the theory: the standard force and moment balances, the microforce balance, and the dissipation inequality. A detailed treatment of the subject can be found elsewhere (see, for example, [2], [4], [5]).

Standard Force System

We characterize the standard force system by the first Piola-Kirchhoff stress $\mathbf{S}$ and by body force per unit volume[1] $\mathbf{b}$, both measured in the reference configuration. Then, the standard force and moment balances are, respectively,

$$\begin{aligned} &\int_{\partial\mathcal{P}} \mathbf{S}\mathbf{n}\, \mathrm{dA} + \int_{\mathcal{P}} \mathbf{b}\, \mathrm{dV} = \mathbf{0}, \\ &\int_{\partial\mathcal{P}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{S}\mathbf{n}\, \mathrm{dA} + \int_{\mathcal{P}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{b}\, \mathrm{dV} = \mathbf{0}, \end{aligned} \tag{4}$$

where $\mathcal{P}$ is an arbitrary part of $\mathcal{B}$, $\mathbf{n}$ the unitary exterior normal to the boundary of $\mathcal{P}$ $(\partial\mathcal{P})$, $\mathbf{y}_0$ is an arbitrary spatial point and $\mathbf{a} \times \mathbf{c}$ represents the vectorial product of the vectors $\mathbf{a}$ and $\mathbf{c}$. In local form, the standard force and moment balances are respectively:

$$\begin{aligned} &\mathrm{Div}\, \mathbf{S} + \mathbf{b} = \mathbf{0}, \\ &\mathbf{S}\mathbf{F}^T = \mathbf{F}\mathbf{S}^T, \end{aligned} \tag{5}$$

where Div$\mathbf{A}$ denotes the divergence of the tensor or vector field $\mathbf{A}$.

The working of the standard forces on a part $\mathcal{P}$ is defined by the classical relation:

$$\mathcal{W}_s(\mathcal{P}) = \int_{\partial\mathcal{P}} \mathbf{S}\mathbf{n} \cdot \dot{\mathbf{y}}\, \mathrm{dA} + \int_{\mathcal{P}} \mathbf{b} \cdot \dot{\mathbf{y}}\, \mathrm{dV} = \int_{\mathcal{P}} \mathbf{S} \cdot \dot{\mathbf{F}}\, \mathrm{dV}, \tag{6}$$

where $\mathbf{A} \cdot \mathbf{B} = \mathrm{tr}\left(\mathbf{A}^T\mathbf{B}\right)$, for $\mathbf{A}$ and $\mathbf{B}$ tensors, and $\mathbf{a} \cdot \mathbf{c}$ is the usual internal product for the vectors $\mathbf{a}$ and $\mathbf{c}$. The last equality is obtained by using $(5)_1$.

Microforce System

The microforce system is characterized by the microstress vector ξ, the (scalar) internal microforce π, the (scalar) external microforce μ. The microforce system is constrained by the microforce balance:

$$\int_{\partial\mathcal{P}} \xi \cdot \mathbf{n}\, \mathrm{dA} + \int_{\mathcal{P}} (\mu + \pi)\, \mathrm{dV} = 0, \tag{7}$$

which in local form is:

$$\mathrm{Div}\, \xi + \pi + \mu = 0. \tag{8}$$

The working of the microforces on a part $\mathcal{P}$ is given by:

$$\mathcal{W}_m(\mathcal{P}) = \int_{\partial\mathcal{P}} (\xi \cdot \mathbf{n})\dot{\alpha}\, \mathrm{dA} + \int_{\mathcal{P}} \mu\dot{\alpha}\, \mathrm{dV} = \int_{\mathcal{P}} (\xi \cdot \dot{\mathbf{p}} - \pi\dot{\alpha})\, \mathrm{dV}, \tag{9}$$

where the last equality is obtained by using (8).

[1] Inertia forces are included in $\mathbf{b}$.

Dissipation Inequality

Within the present purely mechanical context, the Second Law, or Dissipation Inequality, takes the form:

$$\overline{\left(\int_{\mathcal{P}} \psi \, \mathrm{dV}\right)}^{\cdot} \leq \mathcal{W}_s(\mathcal{P}) + \mathcal{W}_m(\mathcal{P}), \qquad \text{for each part } \mathcal{P}, \tag{10}$$

where ψ is the free energy per unit referential volume. The corresponding local form is given by

$$\dot{\psi} - \mathbf{S} \cdot \dot{\mathbf{F}} - \xi \cdot \dot{\mathbf{p}} + \pi \dot{\alpha} \leq 0. \tag{11}$$

CONSTITUTIVE THEORY

In what follows, we assume that the external microforce vanishes ($\mu = 0$).

We consider constitutive equations giving ψ, $\mathbf{S}$, ξ and π at any given point and time when

$$\sigma = (\mathbf{F}, \alpha, \mathbf{p}, \dot{\mathbf{F}}, \dot{\alpha}) \tag{12}$$

are known at that point and time, i.e.,

$$\psi = \psi(\sigma), \quad \mathbf{S} = \mathbf{S}(\sigma), \quad \xi = \xi(\sigma), \quad \pi = \pi(\sigma). \tag{13}$$

We make use of the following decompositions for $\mathbf{S}$ and π:

$$\begin{aligned} \mathbf{S} &= \mathbf{S}_e + \mathbf{S}_d, \\ \pi &= \pi_e + \pi_d, \end{aligned} \tag{14}$$

where

$$\mathbf{S}_e = \mathbf{S}(\mathbf{F}, \alpha, \mathbf{p}, \mathbf{0}, 0) \quad \text{and} \quad \pi_e = \pi(\mathbf{F}, \alpha, \mathbf{p}, \mathbf{0}, 0) \tag{15}$$

are the equilibrium stress and the equilibrium microforce whereas $\mathbf{S}_d$ and π_d are the dynamical stress and the dynamical microforce, respectively. Therefore, by using the Coleman-Noll procedure, the dissipation inequality (11) holds if and only if the conditions

$$\frac{\partial \psi}{\partial \dot{\mathbf{F}}} = \mathbf{0}, \quad \frac{\partial \psi}{\partial \dot{\alpha}} = 0, \quad \xi = \frac{\partial \psi}{\partial \mathbf{p}}, \quad \mathbf{S}_e = \frac{\partial \psi}{\partial \mathbf{F}}, \quad \pi_e = -\frac{\partial \psi}{\partial \alpha}, \tag{16}$$

hold together with the reduced dissipation inequality:

$$\mathcal{D} = \mathbf{S}_d \cdot \dot{\mathbf{F}} - \pi_d \, \dot{\alpha} \geq 0. \tag{17}$$

If we define:

$$\mathbf{J} = \begin{bmatrix} \mathbf{S}_d \\ -\pi_d \end{bmatrix} \quad \text{and} \quad \dot{\mathbf{X}} = \begin{bmatrix} \dot{\mathbf{F}} \\ \dot{\alpha} \end{bmatrix}, \tag{18}$$

the reduced dissipation inequality can be written as:

$$\mathcal{D} = \mathbf{J}(\dot{\mathbf{X}}) \cdot \dot{\mathbf{X}} \geq 0. \tag{19}$$

As $\mathbf{J}(\mathbf{0}) = \mathbf{0}$, the most general solution of (19) is:

$$\mathbf{J}(\dot{\mathbf{X}}) = \mathbf{B}\left[\dot{\mathbf{X}}\right] \quad \text{with} \quad \mathbf{B}(\sigma) = \begin{bmatrix} \mathbf{V} & \mathbf{D} \\ \mathbf{E} & \beta \end{bmatrix} \tag{20}$$

positive semi-definite, in the sense that $\mathbf{B}(\dot{\mathbf{X}}) \cdot \dot{\mathbf{X}} \geq 0$ for all $\dot{\mathbf{X}}$. The fourth-order tensor $\mathbf{V}$ is the tensor of viscosities, the second order tensor $\mathbf{D}$ describe the influence of the rate of decohesion on the value of the nonequilibrium stress. The scalar β is the microdamping, and the second order tensor $\mathbf{E}$ describe the influence of the rate of deformation on the value of the nonequilibrium microforce. Thus, from (14), (16), (18) and (20):

$$\begin{aligned} \mathbf{S} &= \frac{\partial \psi}{\partial \mathbf{F}} + \mathbf{V}\dot{\mathbf{F}} + \dot{\alpha}\mathbf{D}, \\ \pi &= -\frac{\partial \psi}{\partial \alpha} - \mathbf{E} \cdot \dot{\mathbf{F}} - \beta \dot{\alpha}. \end{aligned} \tag{21}$$

The second term of the right-hand side of the above equation can be written as

$$\mathbf{E} \cdot \dot{\mathbf{F}} = \delta\dot{\alpha} + c, \tag{22}$$

where

$$\delta = \delta(\sigma) \quad \text{and} \quad c = \mathbf{E}(\mathbf{F}, \alpha, \mathbf{p}, \dot{\mathbf{F}}, 0) \cdot \dot{\mathbf{F}}. \tag{23}$$

To satisfy the reduced dissipation inequality (19), we assume that

$$\mathbf{V}\dot{\mathbf{F}} \cdot \dot{\mathbf{F}} \geq 0, \quad \beta \geq 0, \quad \dot{\alpha}(\mathbf{D} + \mathbf{E}) \cdot \dot{\mathbf{F}} \geq 0, \tag{24}$$

and, from the last inequality, we conclude that

$$c = -\mathbf{D}(\mathbf{F}, \alpha, \mathbf{p}, \dot{\mathbf{F}}, 0) \cdot \dot{\mathbf{F}}. \tag{25}$$

The constitutive equations $(16)_3$, $(21)_2$ and (22) in the microforce balance (8) result in:

$$\gamma\dot{\alpha} = -\frac{\partial\psi}{\partial\alpha} - c + \text{Div}\left(\frac{\partial\psi}{\partial\mathbf{p}}\right) \quad \text{where} \quad \gamma = \beta + \delta, \tag{26}$$

which represents the kinetic equation for α.

SPECIAL THEORY

Now, by specializing the theory just presented, we show how some features of crack propagation, which are motivated by processes on the microscale and by experimental observations, can be introduced. In this respect, we assume that

$$\psi(\mathbf{F}, \alpha, \mathbf{p}) = \alpha W(\mathbf{F}) + f(\alpha) + g(\mathbf{p}). \tag{27}$$

The function $W(\mathbf{F}) \geq 0$ represents the strain energy of undamaged material. As the order parameter is related to the flaw population, the function $\alpha W(\mathbf{F})$ characterizes the degradation of the material properties with flaw accumulation ([1], [6]). The second term $f(\alpha)$, called the bulk free energy, characterizes the energetic favorability of cohesion states of the material. We use a nonsmooth double obstacle potential [7]:

$$f(\alpha) = \phi(\alpha) + \mathbf{I}_{[0,1]}(\alpha), \tag{28}$$

where ϕ is a concave function with $\phi(1) = \phi(0) = 0$ and $\mathbf{I}_{[0,1]}(\alpha)$ is the indicator function:

$$\mathbf{I}_{[0,1]}(\alpha) = \begin{cases} 0 & \text{if} \quad 0 \leq \alpha \leq 1, \\ +\infty & \text{otherwise.} \end{cases} \tag{29}$$

The third term in equation (27) is called gradient energy, responsible for the diffusive behavior of the order paremeter field ([2], [6]):

$$g(\mathbf{p}) = \frac{1}{2}\kappa|\mathbf{p}|^2, \tag{30}$$

where κ is a material constant.

Also, we assume that $\delta \geq 0$ which implies that $\gamma \geq 0$ in equation (26). From now on, we assume that $\gamma > 0$. In equation (23) we assume that $c = c(\dot{\mathbf{F}})$.

With these assumptions, the evolution equation (26) gives

$$\gamma\dot{\alpha} = -W(\mathbf{F}) + Y, \tag{31}$$

where

$$Y = Y(\alpha, \triangle\alpha, \dot{\mathbf{F}}) = -\partial_\alpha f - c + \kappa\triangle\alpha, \tag{32}$$

is the decohesion resistance. The dependence on $\dot{\mathbf{F}}$ and $\triangle\alpha$ takes into account the influences of strain-rate and non-local effects, respectively, on the decohesion resistance Y. From (31) and (32), we have

$$\begin{cases} \dot{\alpha} > 0 & \text{if} \quad W(\mathbf{F}) < Y, \\ \dot{\alpha} = 0 & \text{if} \quad W(\mathbf{F}) = Y, \\ \dot{\alpha} < 0 & \text{if} \quad W(\mathbf{F}) > Y. \end{cases} \tag{33}$$

The first condition corresponds to the process of healing of microcracks whereas the third condition corresponds to the nucleation and growth of microcraks. If $Y > 0$ we can have either healing ($W(\mathbf{F}) < Y$) or damaging ($W(\mathbf{F}) > Y$). If $Y < 0$, healing is impossible and damaging occurs even if $W(\mathbf{F}) = 0$, which defines the failure of the material.

We specialize the model still further by neglecting non-local effects. In this case, $Y = Y(\dot{\mathbf{F}}, \alpha)$. For each fixed strain-rate, we define α_C in $(0, 1)$ as the solution, if it exists, of the equation $Y = 0$. Thus, we conclude that:

- For a fixed strain-rate, the maximum resistance is attained when $\alpha = 1$;
- If $c < 0$ strain-rate effects increase the resistance of the material;
- If $c > 0$ strain-rate effects decrease the resistance of the material;
- If $\alpha < \alpha_C$, there is no resistance against the decohesion and the material fails.

The following features are derived in our model:

- Criterion for the nucleation of flaw: $W(\mathbf{F}) > Y(\dot{\mathbf{F}}, 1)$;
- Criterion for the growth of flaws: $W(\mathbf{F}) > Y(\dot{\mathbf{F}}, \alpha)$;
- Criterion for the definition of fracture based on attainment of the critical density α_C.

These criteria are the base for dynamic fracture models developed by Zhurkov [8], Curran et al. [9], and Ravi-Chandar and Yang [10].

We observe that the above conditions are not a priori assumptions. Instead, they emerge from the framework just presented.

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