CRACK NUCLEATION SENSITIVITY ANALYSIS

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Abstract. *A simple analytical expression for crack nucleation sensitivity analysis is proposed relying on the concept of topological derivative and applied within a two-dimensional linear elastic fracture mechanics theory. In particular, the topological asymptotic expansion of a shape functional associated to the total potential energy together with a Griffith-type surface energy of an elastic cracked body is calculated. As the main results we derive a crack nucleation criterion based on the topological derivative and a criterion for determining the direction of crack growth based on the topological gradient. The proposed methodology leads to an axiomatic approach of crack nucleation sensitivity analysis.*
Keywords: *topological asymptotic analysis, topological derivative, crack nucleation, brittle fracture*

1. INTRODUCTION

In this paper we propose a general exact analytical expression for crack nucleation sensitivity analysis, where sensitivity is a scalar field that measures how the elastic energy (and in general any chosen shape functional) changes when a small crack is introduced at an arbitrary point of the domain. Its analytical formula is derived by making use of the concept of *topological asymptotic expansion*. In particular, we propose a tool for crack nucleation and crack growth analysis in linear elastic bodies, based on the notions of *topological derivative* and *topological gradient*. In general, the mathematical notion of topological derivative (Céa et al. (2000); Sokołowski and Żochowski (1999)) provides the closed form exact calculation of the sensitivity of a given shape functional with respect to infinitesimal domain perturbations such as the insertion of voids, inclusions, source term or, in this case, a crack. The concept of topological derivative is an extension of the classical notion of derivative. It has been rigorously introduced by Sokołowski and Żochowski (1999) in the context of shape optimization for two-dimensional heat conduction and elasticity problems. In their pioneering paper, these authors have considered domains topologically perturbed by the introduction of a hole subjected to homogeneous Neumann boundary condition. Since then, the notion of topological derivative has proved extremely useful in the treatment of a wide range of problems and has become a subject of intensive research. Its use in the context of topology optimization of load bearing structures (Allaire et al. (2005, 2007); Amstutz and Andrä (2006); Burger et al. (2004); Lee and Kwak (2008); Novotny et al. (2005, 2007)), inverse problems (Feijóo (2004); Amstutz et al. (2005); Masmoudi et al. (2005)) and image processing (Auroux et al. (2007); Belaid et al. (2008); Hintermüller (2005); Larrabide et al. (2008)) are among the main applications of this analytical tool. Concerning the theoretical development on the asymptotic analysis of PDE solutions and topological derivation of shape functionals, the reader may refer for instance to the books by Ammari and Kang (2004) and paper by Nazarov and Sokołowski (2003), respectively. As main results of this paper we have the following contributions:

1. A crack nucleation criterion based on the topological derivative
2. A nucleation result linking the maximal dissipation, vanishing mode II, and maximal stress criteria (which generally do not agree with each other)
3. An alternative proof of the brutal crack nucleation in Griffith's setting.

2. THE MECHANICAL MODEL

Let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$, with smooth boundary $\partial\Omega = \Gamma_N \cup \Gamma_D$ ($\Gamma_N \cap \Gamma_D = \varnothing$), submitted to volume forces b, surface loads q on Γ_N and prescribed displacement h on Γ_D. In our model, the volume forces b will eventually be neglected. Let us also consider a topologically perturbed domain Ω_ε containing a small straight crack γ_ε with endpoints $\hat{x}$ and x^*, and where the parameter ε is a small positive scalar defining the size of the topological perturbation. Symbol n will designate the outward unit normal vector to $\partial\Omega_\varepsilon$. In order to formulate the equilibrium in plane stress and strain linear elasticity as related to the original and perturbed problems, the constitutive relations for linear elastic isotropic materials will be considered. Strain and stress are defined by

$$\nabla^s\xi := \frac{1}{2}\left(\nabla\xi + \nabla\xi^T\right) \qquad \text{and} \qquad \sigma(\xi) = C\nabla^s\xi\ , \qquad \text{with} \qquad C = 2\mu I\!I + \lambda\left(I \otimes I\right)\ , \tag{1}$$

respectively, where ξ represents an admissible displacement field and C the (symmetric) isotropic elasticity tensor. In addition, μ and λ are the Lamé coefficients, that is

$$\mu = \frac{E}{2(1+\nu)}, \qquad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \qquad \text{and} \qquad \lambda = \lambda^* = \frac{\nu E}{1-\nu^2} \ , \tag{2}$$

with E denoting the Young's modulus, ν the Poisson's ratio and λ^* the particular case for plane stress, while I and $\mathbb{I}$ denote the second and fourth order identity tensors, respectively.

2.1 Unperturbed problem

Let us consider an elastic body represented by Ω, which is in equilibrium if the following variational problem holds: find the displacement field $u \in \mathcal{U}$, such that

$$\int_\Omega \sigma(u) \cdot \nabla^s \eta = \int_\Omega b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \qquad \forall \eta \in \mathcal{V} \ , \tag{3}$$

where $\sigma(u) = C\nabla^s u$, $\mathcal{U}$ is the set of admissible displacements and $\mathcal{V}$ the space of admissible variations, which are respectively defined, for $b \in L^2(\Omega)$ and $h, q \in L^2(\partial\Omega)$, as

$$\mathcal{U} := \left\{ u \in H^1(\Omega) : u|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V} := \left\{ \eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0 \right\} \ . \tag{4}$$

The above variational problem has a unique solution and corresponds to the weak formulation of the momentum conservation law with appropriate boundary conditions, namely

$$\left\{ \begin{array}{rcll} -\operatorname{div}(\sigma(u)) & = & b & \text{in} \quad \Omega \\ \sigma(u) & = & C\nabla^s u & \\ u & = & h & \text{on} \quad \Gamma_D \\ \sigma(u)n & = & q & \text{on} \quad \Gamma_N \end{array} \right. , \tag{5}$$

where n is the outward unit normal vector to the boundary $\partial\Omega$.

2.2 Perturbed problem

Let us now consider an elastic cracked body represented by $\Omega_\varepsilon = \Omega \setminus \gamma_\varepsilon$, where $\gamma_\varepsilon \subset \overline{\Omega}$ represents a straight crack of lengh ε. Two distinct situations will be analysed (cf. Fig. 1). In the first case, the crack nucleates at an interior point $\hat{x} \in \Omega$ and grows symmetrically in the direction e. Thus, $\gamma_\varepsilon = [x_A^*; x_B^*] \subset \Omega$, where x_A^* and x_B^* are the crack tips. In this case, since the size ε of the crack is a small parameter, and will eventually tend to zero, the stress distribution around both crack extremities x_A^* and x_B^* are assumed to coincide. This assumption amounts to a symmetry condition with respect to the plane orthogonal to the crack at its mid-point. Alternatively, the crack initializes at a boundary point $\hat{x} \in \partial\Omega$ and grows in the direction e oriented by the angle β defined with respect to the direction of n. Thus, $\gamma_\varepsilon = [\hat{x}; x^*] \subset \overline{\Omega}$, where x^* is the crack tip.

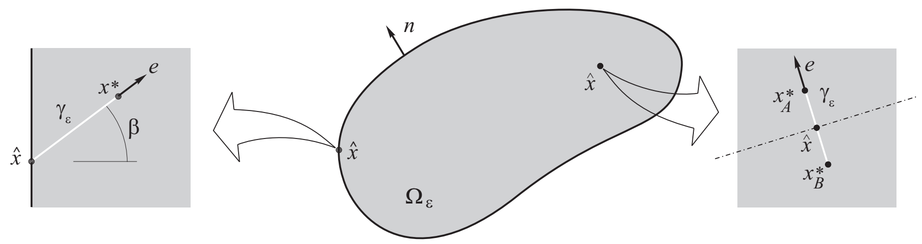


Figure 1. Elastic cracked body represented by the domain Ω_ε.

If the cracked body is in equilibrium, then the following variational problem must be satisfied: find the displacement field $u_\varepsilon \in \mathcal{U}_\varepsilon$, such that

$$\int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \eta = \int_{\Omega_\varepsilon} b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \qquad \forall \eta \in \mathcal{V}_\varepsilon \ , \tag{6}$$

where $\sigma(u_\varepsilon) = C\nabla^s u_\varepsilon$, $\mathcal{U}_\varepsilon$ is the set of admissible displacements and $\mathcal{V}_\varepsilon$ the space of admissible variations, which are respectively defined, for $b \in L^2(\Omega_\varepsilon)$ and $h, q \in L^2(\partial\Omega)$, as

$$\mathcal{U}_\varepsilon := \left\{ u_\varepsilon \in H^1(\Omega_\varepsilon) : u_\varepsilon|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V}_\varepsilon := \left\{ \eta \in H^1(\Omega_\varepsilon) : \eta|_{\Gamma_D} = 0 \right\} \ . \tag{7}$$

The above variational problem is known to have a unique solution, and is precisely the weak formulation of the momentum conservation law with appropriate boundary conditions, namely

$$\left\{\begin{array}{rcll} -\operatorname{div}(\sigma(u_\varepsilon)) & = & b & \text{in} \quad \Omega_\varepsilon \\ \sigma(u_\varepsilon) & = & C\nabla^s u_\varepsilon & \\ u_\varepsilon & = & h & \text{on} \quad \Gamma_D \\ \sigma(u_\varepsilon)n & = & q & \text{on} \quad \Gamma_N \\ \sigma(u_\varepsilon)n & = & 0 & \text{on} \quad \gamma_\varepsilon \end{array}\right. , \tag{8}$$

where n is the outward unit normal vector to the boundary $\partial\Omega_\varepsilon$. The solution to (8) is known to minimize

$$\mathfrak{J}_{\Omega_\varepsilon}(v) = \frac{1}{2}\int_{\Omega_\varepsilon} \sigma(v)\cdot\nabla^s v - \int_{\Omega_\varepsilon} b\cdot v - \int_{\Gamma_N} q\cdot v \ , \tag{9}$$

whose minimal value $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is recognized as the total potential energy of the cracked body. This minimal property of $\mathfrak{J}_{\Omega_\varepsilon}$, namely equation (9) is a simple energetical criterion for determining the displacement in the cracked body. Of course it is by far insufficient from a mechanical viewpoint, since it does not consider any energetical contribution of the (infinitesimal) crack. In fact, let us observe that for any crack, $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) \leq \mathfrak{J}_{\Omega_\varepsilon}(u) = \mathfrak{J}_{\Omega}(u)$, since u is a candidate with vanishing jump for the minimum problem (9) on Ω_ε. Physically, there should be at least a competition between the above decrease of total potential energy due to the presence of a crack, and an increase fo a surface energy concentrated on the crack modelling the energetical cost for increasing the crack size. Accordingly, the so-called Griffith's and Barenblatt's-type variational models are discussed by Bourdin et al. (2008) with a view to determining crack initiation and evolution. Let us presice that these two models account, respectively, for the presence, or not, of cohesive forces between the crack lips, and in such respect provide distinct initiation criteria.

In this paper, we show how the shape functional (9) can provide some relevant information as soon as initiation of a single crack is concerned. In fact, the energy (9) is the simplest case addressed by our method. Griffith's or Barenblatt's-type surface energies, and in general any refinement of (9), provided it admits a topological derivative and for which an appropriate asymptotic analysis is required, can be considered within this sensitivity analysis. One example of crack nucleation with Griffith's-type surface energy will be addressed in section 5.

3. TOPOLOGICAL ASYMPTOTIC ANALYSIS OF THE TOTAL POTENTIAL ENERGY

Let $\psi(\cdot)$ be a shape functional defined over a certain class of domains with sufficient regularity and assume that the following expansion exists

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f(\varepsilon)\, D_T\psi + o(f(\varepsilon)) \ , \tag{10}$$

where $\psi(\Omega)$ is the functional evaluated for the given original domain and $\psi(\Omega_\varepsilon)$ for a perturbed domain obtained by introducing a topological perturbation of size ε. In addition, $f(\varepsilon)$ is a so-called regularizing function defined such that $f(\varepsilon) \to 0^+$ with $\varepsilon \to 0^+$, which depends on the asymptotic behavior of the problem under analysis, while the term $o(f(\varepsilon))$ contains all terms of higher order in $f(\varepsilon)$.

Expression (10) is named the *topological asymptotic expansion* of ψ. The term $D_T\psi$ is defined as the *topological derivative* of ψ at the unperturbed (original) domain Ω. The term $f(\varepsilon)D_T\psi$ is a correction of first order in $f(\varepsilon)$ to the functional $\psi(\Omega)$ to obtain $\psi(\Omega_\varepsilon)$. Nevertheless this definition of the topological derivative is extremely general, and we point out that expansion (10) cannot in general be obtained by conventional means since Ω_ε and Ω do not share the same topology.

Among the methods for calculation of the topological derivative currently available in the literature, we here adopt the methodology described in Novotny et al. (2003), whereby the topological derivative is obtained as the limit

$$D_T\psi = \lim_{\varepsilon\to 0}\left(\frac{1}{f'(\varepsilon)}\frac{d}{d\varepsilon}\psi(\Omega_\varepsilon)\right) \ . \tag{11}$$

The derivative of the shape functional $\psi(\Omega_\varepsilon)$ with respect to the parameter ε denotes precisely the sensitivity of ψ – in the classical sense (Sokołowski and Zolésio (1992)) – to the introduction of the perturbation γ_ε. This term is classically termed *the shape derivative*. The advantage of this last definition for the topological derivative is that the whole mathematical framework (and results) developed for the shape sensitivity analysis can be used to compute the topological derivative. This feature was shown by Novotny et al. (2003) for circular holes and it is now extended when the domain is perturbed by introducing a small crack.

3.1 Application to cracked bodies

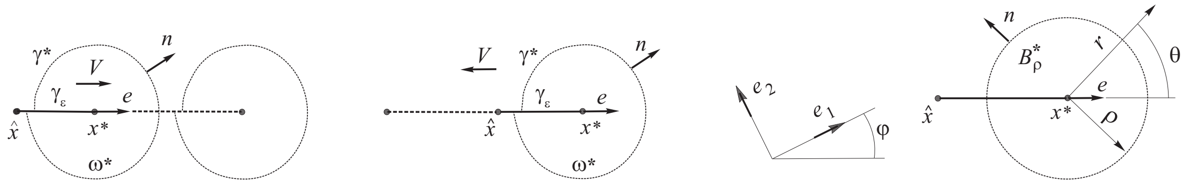
It is assumed that the infinitesimal crack γ_ε remains straight during the growth process (see Fig. 2). Moreover, since the derivative of the shape functional $\psi(\Omega_\varepsilon)$ with respect to the parameter ε means the sensitivity of ψ when the straight crack γ_ε grows, an appropriated shape change velocity field has to be defined. Thus, let us consider an uncracked control volume ω^*, with boundary γ^*, containing the crack tip, i.e. such that $x^* \in \omega^*$. Then, we can define its cracked counterpart as $\omega^*_\varepsilon = \omega^* \setminus \gamma_\varepsilon$. From these elements, the following kinematically admissible *shape change velocity* sets are introduced

$$\mathcal{M} := \{V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega,\ V \cdot n = 0 \text{ in neighb. of } x^* \text{ on } \gamma_\varepsilon\} \tag{12}$$

$$\mathcal{M}_1 := \left\{V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega,\ V = e \text{ in } \overline{\omega^*_\varepsilon}\ \right\}\ , \tag{13}$$

$$\mathcal{M}_2 := \left\{V \in C^\infty(\Omega_\varepsilon) : V = -e \text{ on } \partial\Omega,\ V = 0 \text{ in } \overline{\omega^*_\varepsilon}\ \right\}\ , \tag{14}$$

where e is a constant unit vector aligned with the crack. Therefore, a kinematically admissible velocity field V (i.e., belonging to $\mathcal{M}_1$ or $\mathcal{M}_2$) simulates a crack growth in the direction e.



(a) $V \in \mathcal{M}_1$ (b) $V \in \mathcal{M}_2$ (c) Polar coordinate system (r, θ)

Figure 2. Shape change velocity field.

3.2 Shape derivative calculation

The concept of energy release rate, introduced in the work of Griffiths (1921), represents the rate of change, with respect to crack growth, of the total potential energy available for fracture. As a matter of fact, this concept plays an important role in the mechanical modelling of cracked bodies in linear elastic fracture mechanics. In the work of Feijóo et al. (2000) a systematic methodology was presented in order to obtain the expression of energy release rate in cracked bodies based on shape sensitivity analysis. In order to keep this presentation self-contained, we will restate the equivalence between the concept of energy release rate (Feijóo et al. (2000)) and the shape sensitivity analysis of the functional

$$\psi(\Omega_\varepsilon) := \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - \int_{\Omega_\varepsilon} b \cdot u_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon\ , \tag{15}$$

where the first term represents the energy stored in the linear elastic cracked body, while the second and third terms represent the work done by the body and surface loads, respectively.

In order to compute the shape derivative of $\psi(\Omega_\varepsilon)$, it is convenient to introduce an analogy to classical continuum mechanics where the shape change velocity field V is identified with the classical velocity field of a deforming continuum and ε is identified as a time parameter (see e.g. the book by Gurtin (1981) or, for analogies of this type in the context of shape sensitivity analysis, of Sokołowski and Zolésio (1992)). The following notation is introduced:

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) := \left\langle \frac{\partial}{\partial\Omega_\varepsilon}\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon), V \right\rangle = \frac{d}{d\varepsilon}\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)\ , \tag{16}$$

according to the definition of the shape change velocity sets $\mathcal{M}_1$ (13) or $\mathcal{M}_2$ (14) to which the velocity field V belongs.

Proposition 1 (First form of the shape derivative)**.** *Let $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the functional defined by (15). Then, its derivative with respect to the small parameter ε can be written as*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot V\ , \tag{17}$$

where V is any shape change velocity field belonging to $\mathcal{M}$, while Σ_ε is a generalization of the classical Eshelby momentum-energy tensor (Eshelby (1975); Gurtin (2000)), given by

$$\Sigma_\varepsilon = \frac{1}{2}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)I - \nabla u_\varepsilon^T \sigma(u_\varepsilon)\ . \tag{18}$$

The above shape derivative expression shows a surface integral. Without assuming a vanishing normal velocity field at the crack tip, the following expression of the shape derivative as given by an integral over the cracked domain, is obtained.

Proposition 2 (Second form of the shape derivative)**.** *Let $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the functional defined by (15). Then, the derivative of the functional $\mathfrak{J}_{\Omega_\varepsilon}$ with respect to the small parameter ε is given by*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla V\ , \tag{19}$$

where V is any shape change velocity field belonging to $\mathcal{M}$ and Σ_ε is given by (18).

By taking into account Propositions 1 and 2, the divergence-free property of the Eshelby tensor can immediately be proved in the following sense.

Corollary 3 (Conservation law)**.** *The Eshelby tensor Σ_ε is a divergence-free tensor field away from the crack tip.*

Proposition 4 (Rice integral)**.** *For any control volume ω^* containing the crack tip x^*, with boundary γ^*, the shape derivative of the total potential energy for a rectilinear variation in the direction e of a crack of lengh ε reads*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n = e \cdot \int_{\gamma^*} \Sigma_\varepsilon n \; , \tag{20}$$

where Σ_ε is given by (18).

The shape derivative of the total potential energy might be interpreted as minus energy release rate G_ε due the crack growth. In addition, the above result shows that, for a smooth enough shape change velocity field V, the expression for the energy release rate is independent of the value of V at the interior of the domain Ω_ε, and writes

$$G_\varepsilon = -\alpha \dot{\mathfrak{J}}_{\Omega_\varepsilon} = \alpha e \cdot \int_{\gamma^*} \Sigma_\varepsilon n = \alpha e \cdot \left(\lim_{\rho \to 0} \int_{\partial B_\rho^*} \Sigma_\varepsilon n \right) = \alpha e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n \; , \tag{21}$$

where B_ρ^* is any ball of radius $\rho > 0$ centered at the crack tip x^* (see Fig. 2(c)) and α is the number of crack extremities, namely $\alpha = 1$ or 2 for $\hat{x} \in \partial\Omega$ and $\hat{x} \in \Omega$, respectively. Let us mention that the energy release rate classically coincide with the Rices's integral (Rice (1968)). It turns out that (21) also provides the definition of the configurational force (cf. Gurtin (2000)) acting at the crack tip x^*, together with the relation between force, velocity and dissipation, i.e.,

$$g_\varepsilon^* = \lim_{\rho \to 0} \int_{\partial B_\rho^*} \Sigma_\varepsilon n \qquad \text{and} \qquad \dot{\mathfrak{J}}_{\Omega_\varepsilon} = -g_\varepsilon^* \cdot e \; . \tag{22}$$

3.3 Expressions of the topological derivatives

The aim of this work is to analyse the energetical effect of infinitesimal crack nucleation at $\hat{x}$ in a certain direction e. More precisely, we shall determine the optimal $\hat{x}$ and e in view to decrease at most the potential energy of the elastic cracked body Ω_ε. This will be achieved by calculating the so-called topological derivative of the total potential energy associated to a crack located at $\hat{x}$ in the direction e, as presented in the previous sections. From equations (11) and (22) the topological derivative is introduced as

$$\texttt{TOPOLOGICAL DERIVATIVE} \qquad D_T\psi = -\lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} g_\varepsilon^* \cdot e. \tag{23}$$

This expression of the topological derivative for crack nucleation is interpreted as a diretional derivative, thereby identifying the associated topological gradient $G_T\psi$ as

$$\texttt{TOPOLOGICAL GRADIENT} \qquad G_T\psi = -\lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} g_\varepsilon^*. \tag{24}$$

From an asymptotic analysis around the crack tip as reported in Lemaitre and Chaboche (1988), the above topological derivative gradient expressions can be found.

Indeed, it is known that the displacement field u_ε can be written in terms of the so-called *stress intensity factors (SIF)* K_{I} and K_{II} associated to mode I and II of crack opening. Let us recall that these modes refer to the non-vanishing displacement jump components at the crack, i.e., mode I refers to the case in which $[u_\varepsilon] \cdot n \neq 0, [u_\varepsilon] \cdot e = 0$, while the reverse equalities define mode II. Moreover, the SIF depend on the stress tensor $\sigma(u)$ evaluated far from the crack tip, where u is the solution associated to the original domain Ω without crack, and on the crack orientation e. It should however be noted that the SIF are usually given as functions of the "stress at infinity" in the canonical problem posed in the infinite medium, but also on the geometry of Ω and of the pre-existing crack of length $\varepsilon > 0$ such as orientation, or curvature. Moreover, at any surface or bulk crack initiation point $\hat{x}$, the displacement u_ε is decomposed into a regular term independent of ε and a term in $\sqrt{\varepsilon}$, this decomposition being valid up to $o(\sqrt{\varepsilon})$-terms. In the sequel, asymptotic expansions in a polar coordinate system (r, θ) centered at $\hat{x} \in \Omega$ and aligned with the crack (see Fig. 2(c)) are considered. In particular, the displacement is written as

$$u_\varepsilon = u_\varepsilon^r(r, \theta) e_r + u_\varepsilon^\theta(r, \theta) e_\theta \; , \tag{25}$$

where $\{e_r, e_\theta\}$ denote the polar base located at the crack tip, with $-\pi \leq \theta < \pi$. Furthermore, the results will be given explicitly for plane stress and plane strain and in the absence of body forces.

3.3.1 Plane stress problem

For plane stress problem, we have the following asymptotic expansion for the solution u_ε

- for the mode I

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\,(3-\nu-(1+\nu)\cos\theta)\cos(\theta/2)\ , \tag{26}$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(3-\nu-(1+\nu)\cos\theta)\sin(\theta/2)\ , \tag{27}$$

- for the mode II

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\,(3\nu-1+3(1+\nu)\cos\theta)\sin(\theta/2)\ , \tag{28}$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\,(5+\nu-3(1+\nu)\cos\theta)\cos(\theta/2)\ , \tag{29}$$

where $K_{\mathrm{I}}, K_{\mathrm{II}}$ are the SIF given in terms of the background solution u (let us precise that a small mistake in Lemaitre and Chaboche (1988) has been here corrected). For fixed ε the contour integral in (22) can be taken arbitrarily close to the crack tip, and hence expressions (26)-(29) can be used to evaluate the shape derivative. It results that the configuration force g_ε^* shows to be proportional to ε, providing the expression of f, namely $f(\varepsilon)=\pi\varepsilon^2$, in such a way that, by letting $\varepsilon\to 0$, the expressions (23) of the topological derivative and (24) of the topological gradient becomes

$$D_T\psi(u,e) = -\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) \quad \text{and} \quad G_T\psi(u,e) = -\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right)e\ , \tag{30}$$

respectively. Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) + o(\varepsilon^2)\ . \tag{31}$$

3.3.2 Plane strain problem

For plane strain problem, we have the following asymptotic expansion for the solution u_ε

- for the mode I

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)\,(3-4\nu-\cos\theta)\cos(\theta/2)\ , \tag{32}$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)(3-4\nu-\cos\theta)\sin(\theta/2)\ , \tag{33}$$

- for the mode II

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)\,(4\nu-1+3\cos\theta)\sin(\theta/2)\ , \tag{34}$$

$$u_\varepsilon^\theta(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)\,(4\nu-5+3\cos\theta)\cos(\theta/2)\ , \tag{35}$$

where $K_{\mathrm{I}}, K_{\mathrm{II}}$ are the SIF given in terms of the background solution u (cf. Lemaitre and Chaboche (1988)). Thus, from the above expansions, we can identify function $f(\varepsilon)=\pi\varepsilon^2$ and calculate the limit $\varepsilon\to 0$ in (23) and (24), that is

$$D_T\psi(u,e) = -\alpha\frac{1-\nu^2}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) \quad \text{and} \quad G_T\psi(u,e) = D_T\psi(u,e)e\ . \tag{36}$$

Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2\alpha\frac{1-\nu^2}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) + o(\varepsilon^2)\ . \tag{37}$$

4. MINIMAL TOPOLOGICAL DERIVATIVE AS A CRACK NUCLEATION CRITERION

The above analysis provides a new feature, since for cracks of vanishing length, a precise notion of topological derivative – given by equations (30) and (36)) has been introduced. Moreover this derivative is evaluated from the sole knowledge of the asymptotic behaviour of the solution near the crack. Let us point out that as soon as the total potential energy $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is concerned, the explicit expression (30) or (36) shows its topological derivative as always non-positive, meaning that the presence of a crack of any length anywhere in Ω will provide a lower total potential energy as compared to the uncracked body. This property is completely natural since nucleation means extending the class of candidates for the minimization of (9) with those candidates that might jump across the crack lips. To that extend, the topological derivation has not brought significant insight to the nucleation issue. It results that from the notion of topological derivative, the principle of maximal dissipation or, equivalently, of minimal topological derivative, do provide a crack nucleation criterion. In fact, (30) and (36) do provide an explicit criterion for the determination of the weakest zones in Ω with respect to crack initiation, in the sense that the nucleation points $x^\star$ and orientation $e(\varphi^\star)$ can be sought such that

$$\texttt{NUCLEATION CRITERION} \qquad D_T\psi(x^\star, e(\varphi^\star)) = \min_{x\in\Omega, \varphi\in[0;2\pi[} D_T\psi(x, e(\varphi)), \tag{38}$$

where φ is the angle between e and e_1 with $\{e_1, e_2\}$ a local base at x.

4.1 Case 1: bulk crack initiation

Let us fix $x \in \Omega$, and take $\alpha = 2$ in order to account for the crack symmetry property. According to the classical expressions of the SIF given for the canonical problem (see Lemaitre and Chaboche (1988)), it results that

$$K_{\mathrm{I}} = \sigma(u)e^\perp \cdot e^\perp \qquad \text{and} \qquad K_{\mathrm{II}} = \sigma(u)e \cdot e^\perp , \tag{39}$$

where u is the solution to the background problem (without crack). Hence, the topological derivative writes

- for plane stress, as

$$D_T\psi = -\frac{1}{2E}\left[(\sigma(u)e^\perp \cdot e^\perp)^2 + (\sigma(u)e \cdot e^\perp)^2\right] , \tag{40}$$

- and for plane strain, as

$$D_T\psi = -\frac{1-\nu^2}{2E}\left[(\sigma(u)e^\perp \cdot e^\perp)^2 + (\sigma(u)e \cdot e^\perp)^2\right] . \tag{41}$$

In any of the two cases, the crack will, according to the above criterion (38), nucleate in a direction that minimizes the topological derivative. Hence, by writing

$$e = (\cos\varphi, \sin\varphi) \qquad \text{and} \qquad e^\perp = (-\sin\varphi, \cos\varphi) , \tag{42}$$

where φ denotes the angle between the crack direction e and the local basis $\{e_1, e_2\}$ located at x (cf. Fig. 2(c)), it suffices to find $\varphi^\star$ such that

$$\varphi^\star := \arg\left\{\max_{0\le\theta<2\pi}\left[\sigma_{11}^2 + 2\sigma_{12}^2 + \sigma_{22}^2 + (\sigma_{22}^2 - \sigma_{11}^2)\cos(2\theta) - 2\sigma_{12}(\sigma_{11}+\sigma_{22})\sin(2\theta)\right]\right\} , \tag{43}$$

which results in

$$\varphi^\star = \pm\frac{1}{2}\arccos\left(\pm\sqrt{\frac{(\sigma_{11}-\sigma_{22})^2}{(\sigma_{11}-\sigma_{22})^2 + 4\sigma_{12}^2}}\right) \tag{44}$$

where σ_{ij} are the components of the stress tensor $\sigma(u)$ in the local system $\{e_1, e_2\}$ and $\varphi^\star$ denotes the angle that maximizes the energy release rate.

According to this topological minimization framework, the so-called "Local Symmetry Principle" (see the pioneering works of Barenblatt and Cherepanov (1961) and Erdogan and Sih (1963), and the recent discussion by Chambolle et al. (2009)), otherwise called "$K_{\mathrm{II}} = 0$" nucleation criterion, instead of being simply postulated, can now be proved.

Proposition 5 ($K_{\mathrm{II}} = 0$ nucleation criterion)**.** *In homogeneous LEFM, the $K_{\mathrm{II}} = 0$ crack nucleation criterion satisfies the property of minimal topological derivative, i.e., of maximal decrease of the total potential energy (9).*

Proof. If $\{e_1, e_2\}$ are the principal direction at x, then the stress $\sigma(u)$ is diagonal,

$$\sigma(u) = \sum_{i=1}^{2} \sigma_i(u)(e_i \otimes e_i) \ ,$$

where e_i are the eigen-vectors associated to the eigen-values $\sigma_i(u)$ (with $\sigma_1 > \sigma_2$) of tensor $\sigma(u)$ evaluated at x, and equation (44) results in $\varphi^\star = 0$ or $\pi/2$. Clearly, since $e_2^\perp = e_1$, the lowest value of the topological derivative is attained for $\varphi^\star = \pi/2$. □

4.2 Case 2: boundary crack initiation

In this case, $\hat{x} \in \partial\Omega$, there is one crack extremity at the boundary, and the other inside the body, i.e. $\alpha = 1$. In addition, the SIF $K_{\rm I}$ and $K_{\rm II}$ are given by (cf. Beghinia et al. (1999))

$$\begin{pmatrix} K_{\rm I} \\ K_{\rm II} \end{pmatrix} = \begin{pmatrix} F_{\rm I}^S & F_{\rm I}^T \\ F_{\rm II}^S & F_{\rm II}^T \end{pmatrix} \begin{pmatrix} \sigma(u)e^\perp \cdot e^\perp \\ \sigma(u)e \cdot e^\perp \end{pmatrix} , \tag{45}$$

where coefficients $F_{\rm I}^S, F_{\rm I}^T$ and $F_{\rm II}^S, F_{\rm II}^T$ depend on the angle β that the crack forms with the normal n. According to the above expressions of the SIF, the topological derivative reads

- for plane stress, as

$$D_T\psi = -\frac{1}{4E}\left[(F_{\rm I}^S\sigma(u)e^\perp \cdot e^\perp + F_{\rm I}^T\sigma(u)e \cdot e^\perp)^2 + (F_{\rm II}^S\sigma(u)e^\perp \cdot e^\perp + F_{\rm II}^T\sigma(u)e \cdot e^\perp)^2\right] , \tag{46}$$

- and for plane strain, as

$$D_T\psi = -\frac{1-\nu^2}{4E}\left[(F_{\rm I}^S\sigma(u)e^\perp \cdot e^\perp + F_{\rm I}^T\sigma(u)e \cdot e^\perp)^2 + (F_{\rm II}^S\sigma(u)e^\perp \cdot e^\perp + F_{\rm II}^T\sigma(u)e \cdot e^\perp)^2\right] . \tag{47}$$

In this case, there are no close representation for the SIF $K_{\rm I}$ and $K_{\rm II}$. However we can find some approximated formulas (see, for instance, Beghinia et al. (1999)), which can be adopted in the calculation of the optimal angle $\varphi^\star$, following exactly the same steps as presented in the previous case.

5. CRACK NUCLEATION UNDER A SIMPLE BULK AND SURFACE ENERGY COMPETITION

It has been mentioned that physically an energy contribution consisting of a line integral over the crack should be added to the elastic (bulk) energy of the cracked body. In order to show how our axiomatic approach can be applied to different types of energy-based shape functionals, let us consider the Griffith's-type surface energy of the form

$$\Xi(\Omega_\varepsilon) = \psi(\Omega_\varepsilon) + C(\gamma_\varepsilon) \quad \text{with} \quad C(\gamma_\varepsilon) = \int_{\gamma_\varepsilon} \kappa(\varepsilon) \ , \quad \text{whose simplest expression is taken as} \quad C(\gamma_\varepsilon) = \tilde{\kappa}\varepsilon \ , \tag{48}$$

where $\tilde{\kappa} > 0$ is the specific (material dependent) surface energy. The solutions to the associated elastic problem, obtained by a global minimization approach (see, e.g., Bourdin et al. (2008)), here satisfy (8). From (48) it follows that the derivative w.r.t. ε of $C(\gamma_\varepsilon)$ is given by

$$\dot{C}(\gamma_\varepsilon) = \tilde{\kappa} > 0 \ . \tag{49}$$

whereby from (31) or (37) and (49) it results that $\Xi(\Omega_\varepsilon)$ admits the following total derivative w.r.t. ε:

$$\dot{\Xi}(\Omega_\varepsilon) = \tilde{\kappa} + O(\varepsilon) \ , \tag{50}$$

From this latter result we have $f_\Xi(\varepsilon) = \varepsilon$ and the expression of the topological derivative of Ξ reads

$$D_T\Xi = \lim_{\varepsilon \to 0}\left(\frac{1}{f_\Xi'(\varepsilon)}\dot{\Xi}(\Omega_\varepsilon)\right) = \tilde{\kappa} > 0 \ . \tag{51}$$

Since the topological derivative of Ξ is always non negative, the surface energy contribution $C(\gamma_\varepsilon) = \tilde{\kappa}\varepsilon$ will always prohibit nucleation.

Proposition 6. *In homogeneous LEFM, according to the topological derivative criterion (38) as applied to (48), there will be no infinitesimal crack nucleation.*

The above property is in fact another proof of a result found in Bourdin et al. (2008) and stating that in the Griffith setting nucleation at defect-free points can only occur brutally, i.e., not infinitesimally. In addition, considering only the case associated with bulk crack nucleation ($\alpha = 2$), the finite critical crack sizes $\varepsilon^\star$ can be explicitely bounded from below. In fact, the topological asymptotic expansion of the shape functional (48) reads

$$\Xi(\Omega_\varepsilon) = \Xi(\Omega) + \varepsilon\tilde{\kappa} + \pi\varepsilon^2 D_T\psi + o(\varepsilon^2) \ . \tag{52}$$

where $D_T\psi$ can be obtained from (31) and (37) for plane stress and plane strain, respectively. Hence, as a result of the balance between potential and surface energy contributions, the following thresholds are found:

$$\text{for plane stress} \quad \varepsilon^\star > \frac{2\tilde{\kappa}E}{\pi K_{\mathrm{I}}^2} \ ; \qquad \text{for plane strain} \quad \varepsilon^\star > \frac{2\tilde{\kappa}E}{\pi(1-\nu^2)K_{\mathrm{I}}^2} \ ; \tag{53}$$

since that, according to Proposition 5, in this case we have $\varphi^\star = \pi/2$ and $K_{\mathrm{II}} = 0$.

6. CONCLUSIONS

In this paper, we mainly provide a simple tool justified by a rigorous mathematical approach, aimed at analysing crack nucleation in various physical models within the class of linear elastic bodies. The proposed crack nucleation criterion is based on the notion of topological asymptotic expansion as applied to a shape functional associated to the total potential energy of an elastic cracked body. The case of surface energy contributions of Griffith-type has also been considered. Most of the result of this paper were previously known by other approaches. However the methodology introduced in this paper is original and permits to prove results which were previously only considered as postulates, or principles. As the main results we have mathematically formulated a crack nucleation criterion based on the topological derivative the topological gradient. The proposed methodology leads to an axiomatic approach which can be used for further analysis of crack growth. In addition, it has the advantage of (i) being rigorously defined, (ii) easily tractable, and (iii) of use in various physical models of fracture. Concerning this latter point, provided the solution to the primal perturbed problem is known with other crack boundary conditions than those of (8) and given its asymptotic expression in terms of the small crack length ε, the proposed framework can be applied, resulting in appropriate nucleation criteria. Moreover, it is clear that other cost function than the potential or Griffith energy can freely be chosen within our setting, thereby providing a family of nucleation criteria, which can be tested and compared by laboratory or numerical experiments.

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