Crack Nucleation Sensitivity Analysis

N. Van Goethem[*,a], A.A. Novotny[b]

[a]*Centro de Matemática e Aplicações Fundamentais CMAF,*
Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal
[b]*Laboratório Nacional de Computação Científica LNCC/MCT*
Coordenação de Matemática Aplicada e Computacional,
Av. Getúlio Vargas 333, 25651-075 Petrópolis - RJ, Brasil

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.

Key words: topological asymptotic analysis, topological derivative, crack nucleation, brittle fracture

1. Introduction

The theory of brittle fracture takes its origin in the work of Griffiths (1921), later pursued by the key theoretical contributions of Irwin (1958), Cherepanov (1979), Erdogan and Sih (1963) and Rice (1968). In the 80ies the work of Lemaitre and Chaboche (1988) paved the way for the numerical simulation of crack evolution (for which we refer to Amestoy and Leblond (1992); Moës et al. (2002a,b); Bourdin et al. (2000) among others).

However the question of the full mathematical justification of brittle fracture only arose about 15 years ago with the work of Francfort and Marigo (1998) and is a continued topic of active research nowadays (see e.g. Bourdin et al. (2008) and Chambolle et al. (2008b)). One of their main contribution was to avoid the specification of a known crack path for crack evolution predictions. Moreover, they focussed on crack obtained by a global minimization approach in a quasi-static setting, but nowadays their original approach is being extended

---

[*]Corresponding author.
  Email address: `vangoeth@ptmat.fc.ul.pt` (N. Van Goethem)

to dynamical crack growth by Bourdin et al. (2009) (see also Song et al. (2008)), while local approaches are addressed from a theoretical viewpoint by, e.g., Knees et al. (2002), and numerically by, e.g., Allaire et al. (2007).

In general, analysis of crack propagation consider an already cracked body Feijóo et al. (2000). However, criteria for crack growth are still discussed in the Mechanical community. The first laboratory experiments of bar extensions appealed to the so-called maximal stress criterion, whereas this criterion failed to predict general cracked bodies where the loads are not aligned with the crack. Therefore, the concept of stress intensity factor (SIF) as a measure of stress in the crack process zones appeared and reached consensus. Some authors, like Sih (1973), instead of rely on a simple critical SIF criterion, have proposed local criteria based on the so-called strain-energy density functions. These local methods are not easily tractable since relying on the permanent re-evaluation of the SIFs for every new cracked body configuration. Other authors, like Irwin and Rice, proposed local crack growth principles based on the notion of *maximal dissipation* at the crack tip. On the other hand, relying on symmetry arguments, Cherepanov (1979) and Erdogan and Sih (1963), have proposed a local growth criterion based on the principle that the crack growths with *vanishing (shearing) mode* II. As shown by Amestoy and Leblond (1992), these variety of criteria are not equivalent, and therefore the continued interest in mathematical approaches is justified (see also the recent contributions of Chambolle et al. (2008a, 2009) and Hakim and Karma (2008)).

Concerning crack nucleation criteria, even less consensus is reached. It is sometimes read that initiation is not the concern of fracture modeling, limited to the growth of existing pre-cracks, while other authors believe that crack evolution and nucleation criteria should be intimately related. Then, the above mentioned growth criteria are usually postulated for crack of finite lengh as well as for infinitesimal cracks, i.e., for nucleation. From a mathematical viewpoint, Francfort, Marigo and co-workers (see also Chambolle et al. (2008b)) have proved some results relating crack initiation to a local measure of singularity, that is, to the presence, or not, of defects in the elastic body under analysis. In particular, they proved that in the absence of defects brittle fracture can only occur brutally, that is, for a minimal crack lenght, and discussed the question of time-continuity of crack paths as related to kinking criteria Chambolle et al. (2009). However, in the work of Knees et al. (2002), it is remarked that the drawback of these global minimization approaches is to predict underevalueted crack initiation times.

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.

2

(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. (2004, 2005, 2007); Amstutz and Andrä (2006); Burger et al. (2004); Lee and Kwak (2008); Novotny et al. (2005, 2007), inverse problems Amstutz et al. (2005); Feijóo (2004); 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.

Let us emphasize that the two latter results cannot be claimed new. Nevertheless, to our knowledge the original contribution of this paper is to establish an *axiomatic approach* for addressing crack nucleation problems, where a precise mathematical notion of nucleation is given. Moreover, the nucleation criterion provided by this approach shows how the principles of maximal dissipation, vanishing mode II, and maximal stress, are understood with respect to crack nucleation. Let us also precise that the specification of a global or local approach is not an *a priori* requirement, and that the – intrinsic local – notion of topological derivative, and derived crack nucleation criterion should eventually be coupled with other tools with a view to crack growth predictions.

The paper is organized as follows. The mechanical model associated to plane stress linear elasticity is described in section 2. The closed formula for the crack nucleation sensitivity analysis is presented in section 3. In particular, we firstly introduce an overview of the topological asymptotic analysis concept and state a method for calculating the topological derivative. The adopted approach is cast within the shape sensitivity analysis setting described by Novotny et al.

(2003). In section 3.1 we extend our theory for cracked bodies. Following the original ideas presented by Feijóo et al. (2000), the shape sensitivity analysis is performed in section 3.2. The calculation of the topological derivative associated to the total potential energy of the cracked body is then presented in section 3.3. Section 4 is dedicated to the interpretation of the obtained topological derivative and gradient. In section 5, another energy criterion, including surface contributions, is analysed within our method. Finally, some concluding remarks are made in section 6.

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

$$\nabla^s \xi := \frac{1}{2} \left(\nabla\xi + \nabla\xi^T \right) \qquad \text{and} \qquad \sigma(\xi) = C\nabla^s\xi , \qquad (2.1)$$

respectively, where ξ represents an admissible displacement field, and C is the (symmetric) isotropic elasticity tensor given by

$$C = 2\mu I\!\!I + \lambda \left(I \otimes I \right) , \qquad (2.2)$$

where μ and λ are the Lamé coefficients, that is

$$\mu = \frac{E}{2(1+\nu)}, \qquad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \qquad \text{and} \qquad \lambda = \lambda^* = \frac{\nu E}{1-\nu^2} , \quad (2.3)$$

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

2.1. Unperturbed problem

Let us consider an elastic body represented by Ω (see fig. 1), which is in equilibrium if the following variational problem holds: find the displacement field $u \in \mathcal{U}$, such that

$$\int_\Omega \sigma(u) \cdot \nabla^s\eta = \int_\Omega b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \qquad \forall\eta \in \mathcal{V} , \qquad (2.4)$$

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

$$\mathcal{U} := \left\{ u \in H^1(\Omega) : u|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V} := \left\{ \eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0 \right\} . \quad (2.5)$$

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

$$\begin{cases} -\operatorname{div}(\sigma(u)) &= b & \text{in} \quad \Omega \\ \sigma(u) &= C\nabla^s u \\ u &= h & \text{on} \quad \Gamma_D \\ \sigma(u)n &= q & \text{on} \quad \Gamma_N \end{cases} , \quad (2.6)$$

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

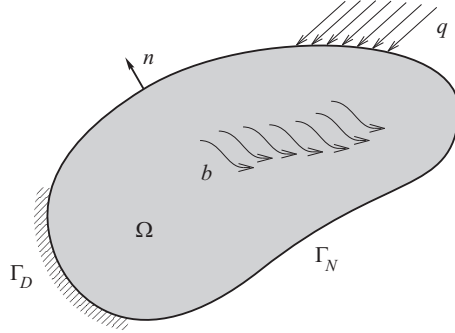

Figure 1: Elastic uncracked body represented by the domain Ω.

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. 2). 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.
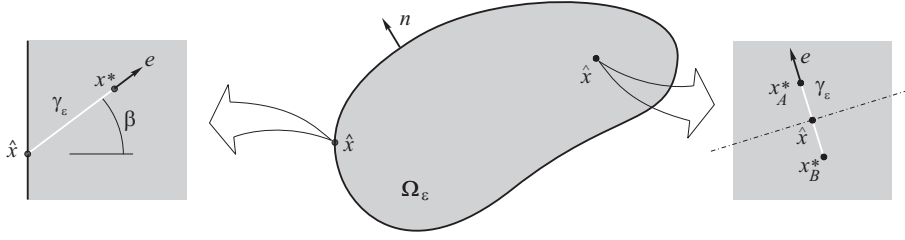
Figure 2: Elastic cracked body represented by the domain Ω_ε.

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

$$\int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \eta = \int_{\Omega_\varepsilon} b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \qquad \forall \eta \in \mathcal{V}_\varepsilon \ , \tag{2.7}$$

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

$$\mathcal{U}_\varepsilon := \left\{ u_\varepsilon \in H^1(\Omega_\varepsilon) : u_\varepsilon|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V}_\varepsilon := \left\{ \eta \in H^1(\Omega_\varepsilon) : \eta|_{\Gamma_D} = 0 \right\} \ . \tag{2.8}$$

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

$$\begin{cases} -\operatorname{div}(\sigma(u_\varepsilon)) &= b & \text{in} & \Omega_\varepsilon \\ \sigma(u_\varepsilon) &= C\nabla^s u_\varepsilon \\ u_\varepsilon &= h & \text{on} & \Gamma_D \\ \sigma(u_\varepsilon)n &= q & \text{on} & \Gamma_N \\ \sigma(u_\varepsilon)n &= 0 & \text{on} & \gamma_\varepsilon \end{cases} , \tag{2.9}$$

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

Let us remark that, since the perturbed domain is non-Lipschitz, its solution, as opposed to (2.6) does not belong to $H^2(\Omega_\varepsilon)$. In particular the displacement provokes unbounded stresses at the crack tip, and is allowed to jump across γ_ε. Let us remark that the tip singularity is due to the inadequacy of the linear elastic model near the crack extremeties. Let us also point out that the last condition in (2.9) amounts to neglect the dynamic effect of cohesive forces between the crack lips, whereas their inter-penetration (i.e., negative normal jump component of the displacement at the crack) is not prohibited in the above model. The latter effect is a classical drawback of linear fracture mechanics, and will not be discussed any further in the sequel.

The solution to (2.9) is known to minimize

$$\mathfrak{J}_{\Omega_\varepsilon}(v) = \frac{1}{2} \int_{\Omega_\varepsilon} \sigma(v) \cdot \nabla^s v - \int_{\Omega_\varepsilon} b \cdot v - \int_{\Gamma_N} q \cdot v \ , \tag{2.10}$$

6

whose minimal value $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ is recognized as the total potential energy of the cracked body.

The above minimal property of $\mathfrak{J}_{\Omega_\varepsilon}$, namely equation (2.10) 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 (2.10) 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 (2.10) can provide some relevant information as soon as initiation of a single crack is concerned. In fact, the energy (2.10) is the simplest case addressed by our method. Griffith's or Barenblatt's-type surface energies, and in general any refinement of (2.10), 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

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f(\varepsilon) D_T \psi + o(f(\varepsilon)) , \qquad (3.1)$$

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

$$\lim_{\varepsilon \to 0^+} f(\varepsilon) = 0 , \qquad (3.2)$$

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 (3.1) 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 (3.1) cannot

7

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); Sokołowski and Żochowski (2001), whereby the topological derivative is obtained as the limit

$$D_T\psi = \lim_{\varepsilon \to 0} \left(\frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\Omega_\varepsilon) \right) . \tag{3.3}$$

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. 3). 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

$$\mathcal{M} \quad := \quad \left\{ V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega, \ V \cdot n = 0 \text{ in neighb. of } x^* \text{ on } \gamma_\varepsilon \right\} \tag{3.4}$$

$$\mathcal{M}_1 \quad := \quad \left\{ V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega, \ V = e \text{ in } \overline{\omega_\varepsilon^*} \right\} , \tag{3.5}$$

$$\mathcal{M}_2 \quad := \quad \left\{ V \in C^\infty(\Omega_\varepsilon) : V = -e \text{ on } \partial\Omega, \ V = 0 \text{ in } \overline{\omega_\varepsilon^*} \right\} , \tag{3.6}$$

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.
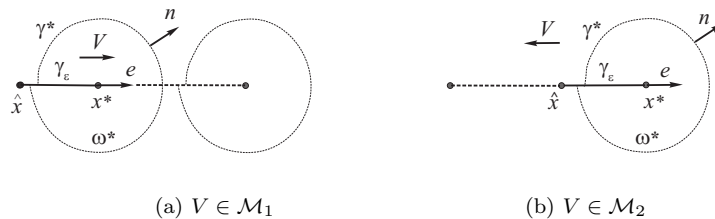
(a) $V \in \mathcal{M}_1$ (b) $V \in \mathcal{M}_2$

Figure 3: 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

$$\psi(\Omega_\varepsilon) := \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - \int_{\Omega_\varepsilon} b \cdot u_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon \ , \qquad (3.7)$$

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:

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) := \left\langle \frac{\partial}{\partial \Omega_\varepsilon} \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon), V \right\rangle = \frac{d}{d\varepsilon} \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) \ , \qquad (3.8)$$

according to the definition of the shape change velocity sets $\mathcal{M}_1$ (3.5) or $\mathcal{M}_2$ (3.6) 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 (3.7). Then, its derivative with respect to the small parameter ε can be written as*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial \Omega_\varepsilon} \Sigma_\varepsilon n \cdot V \ , \qquad (3.9)$$

9

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

$$\Sigma_\varepsilon = \frac{1}{2}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)I - \nabla u_\varepsilon^T \sigma(u_\varepsilon) . \qquad (3.10)$$

PROOF. Let us compute the shape derivative of the functional $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ using the following version for the Reynolds' Transport Theorem (Gurtin (1981); Sokołowski and Zolésio (1992)),

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)' + \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)V \cdot n$$
$$- \int_{\Omega_\varepsilon} b \cdot u_\varepsilon' - \int_{\partial\Omega_\varepsilon}(b \cdot u_\varepsilon)V \cdot n - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon \operatorname{div}_{\partial\Omega}(V) \quad (3.11)$$

where $\operatorname{div}_{\partial\Omega}(V) = (I - n \otimes n) \cdot \nabla V$ is the superficial divergence of the velocity field V. In addition, the prime and the superimposed dot are respectively used to denote the partial (spatial) and the total (material) derivatives with respect to ε. Let us observe that the last term on the RHS of (3.11) vanishes by the definition of the velocity field.

Let us here remark that the cracked body Ω_ε has a singular boundary and hence that usual regularity theorems do not hold at the crack extremities. However it is known from the work of Grisvard (1989) that the solution u_ε writes as a regular $H^2(\Omega_\varepsilon)$-term plus a singular term writing as $u_\varepsilon^s = \Psi_\varepsilon(\theta)r^{1/2}$ where (r, θ) is a system of polar coordinates with pole at the crack tip. Therefore it appears that the second term on the RHS of (3.11) is, because of that singular term, not well-defined at the crack tip, unless $V \cdot n$ vanishes, which is indeed the assumption made on the applied velocity field.

Next, by using the concept of spatial derivative (cf. Gurtin (1981); Sokołowski and Zolésio (1992)), we find that the first term of the above RHS integral can be written as

$$(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)' = 2\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon' = 2\sigma(u_\varepsilon) \cdot (\nabla^s \dot{u}_\varepsilon - \nabla^s(\nabla u_\varepsilon V)) , (3.12)$$

where it is remarked that the material derivative $\dot{u}_\varepsilon$ has the same regularity as u_ε, and that the last term inside the parenthesis, as integrated over Ω_ε, is given a meaning by partial integration and by the property that $\sigma(u_\varepsilon)n$ vanishes along the crack. With the above result, the sensitivity of the functional $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ reads

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)V \cdot n - \int_{\Omega_\varepsilon}\sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V)$$
$$+ \int_{\Omega_\varepsilon} b \cdot \nabla u_\varepsilon V + \int_{\Omega_\varepsilon}\sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} b \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon \quad (3.13)$$

Since $\dot{u}_\varepsilon \in \mathcal{V}_\varepsilon$, the equilibrium equation (2.7) implies that the last three terms of (3.13) vanish, and hence

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\partial\Omega_\varepsilon}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)V \cdot n - \int_{\Omega_\varepsilon}\sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V) + \int_{\Omega_\varepsilon} b \cdot \nabla u_\varepsilon V .$$
$$(3.14)$$

Eventually, using the tensor relation

$$\mathrm{div}(\sigma(u_\varepsilon)(\nabla u_\varepsilon V)) = \sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V) + \mathrm{div}(\sigma(u_\varepsilon)) \cdot \nabla u_\varepsilon V , \qquad (3.15)$$

and the divergence theorem, expression (3.14) can be written as

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot V + \int_{\Omega_\varepsilon} [\,\mathrm{div}(\sigma(u_\varepsilon)) + b\,] \cdot \nabla u_\varepsilon V , \qquad (3.16)$$

and since the stress field $\sigma(u_\varepsilon)$ is in equilibrium, the proof of (3.9) simply results from (2.9).

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 (3.7). Then, the derivative of the functional $\mathfrak{J}_{\Omega_\varepsilon}$ with respect to the small parameter ε is given by*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla V , \qquad (3.17)$$

where V is any shape change velocity field belonging to $\mathcal{M}$ and Σ_ε is given by (3.10).

PROOF. Another version of Reynolds' Transport Theorem (Gurtin (1981); Sokołowski and Zolésio (1992)) provides the identity

$$
\begin{aligned}
\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2} \int_{\Omega_\varepsilon} [(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)^\cdot + (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)\,\mathrm{div}(V)] \\
&\quad - \int_{\Omega_\varepsilon} [b \cdot \dot{u}_\varepsilon + (b \cdot u_\varepsilon)\,\mathrm{div}(V)] - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon\,\mathrm{div}_{\partial\Omega}(V) \quad (3.18)
\end{aligned}
$$

Once again, the last term on the RHS of (3.18) vanishes by the definition of the velocity field. Next, by using the concept of material derivative of a spatial field (Gurtin (1981); Sokołowski and Zolésio (1992)), we find that the first term of the above RHS integral can be written as

$$(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)^\cdot = 2\sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - 2\nabla u_\varepsilon^T \sigma(u_\varepsilon) \cdot \nabla V , \qquad (3.19)$$

which, substituted in (3.18) gives

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla V + \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} b \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon , \quad (3.20)$$

Since $\dot{u}_\varepsilon \in \mathcal{V}_\varepsilon$, and with the equilibrium equation (2.7), the last three terms of (3.20) vanish, thereby proving the result.

11

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.*

PROOF. By applying the divergence theorem to the right hand side of (3.17), we have

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega_\varepsilon} \Sigma_\varepsilon n \cdot V - \int_{\Omega_\varepsilon} \operatorname{div}(\Sigma_\varepsilon) \cdot V \ . \tag{3.21}$$

Since (3.9) and (3.17) hold for any velocity fields in $\mathcal{M}$, it results that

$$\int_{\Omega_\varepsilon} \operatorname{div}(\Sigma_\varepsilon) \cdot V = 0 \quad \forall V \in \mathcal{M} \quad \Rightarrow \quad \operatorname{div}(\Sigma_\varepsilon) = 0 \text{ a.e. in } \Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*} \ . \tag{3.22}$$

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*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n = e \cdot \int_{\gamma^*} \Sigma_\varepsilon n \ , \tag{3.23}$$

where Σ_ε is given by (3.10).

PROOF. Let us define $\hat{\gamma}_\varepsilon = \gamma_\varepsilon \cap (\Omega \setminus \overline{\omega^*})$. Since $\operatorname{div}(\Sigma_\varepsilon) = 0$ in $\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}$ it results that the shape derivative of the total potential energy given by (3.17), after integrating by parts, becomes

$$\begin{aligned}
\dot{\mathfrak{J}}_{\Omega_\varepsilon} &= \int_{\Omega_\varepsilon} \Sigma_\varepsilon \cdot \nabla V = \int_{\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}} \Sigma_\varepsilon \cdot \nabla V + \int_{\omega_\varepsilon^*} \Sigma_\varepsilon \cdot \nabla V \\
&= \int_{\partial\Omega} \Sigma_\varepsilon n \cdot V + \int_{\hat{\gamma}_\varepsilon} \Sigma_\varepsilon n \cdot V - \int_{\gamma^*} \Sigma_\varepsilon n \cdot V + \int_{\omega_\varepsilon^*} \Sigma_\varepsilon \cdot \nabla V \ . \tag{3.24}
\end{aligned}$$

Let us consider the velocity field $V \in \mathcal{M}_2$ given by (3.6) in the above result (3.24), which implies

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega} \Sigma_\varepsilon n \cdot V + \int_{\hat{\gamma}_\varepsilon} \Sigma_\varepsilon n \cdot V \quad \text{with} \quad V \in \mathcal{M}_2 \ . \tag{3.25}$$

Taking into account that $n \perp V$ on $\hat{\gamma}_\varepsilon$ and considering that $\sigma(u_\varepsilon)n = 0$ on $\hat{\gamma}_\varepsilon$, equation (3.25) becomes

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega} \Sigma_\varepsilon n \cdot V = -e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n \quad \text{with} \quad V \in \mathcal{M}_2 \ . \tag{3.26}$$

If, in turn, the velocity field $V \in \mathcal{M}_1$ given by (3.5) is inserted in (3.24), it results, by using the same arguments as above, that

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = -\int_{\gamma^*} \Sigma_\varepsilon n \cdot V = -e \cdot \int_{\gamma^*} \Sigma_\varepsilon n \quad \text{with} \quad V \in \mathcal{M}_1 \ . \tag{3.27}$$

On the other hand, by considering (3.22), it can be shown that both (3.26) and (3.27) are actually equivalents, namely

$$
\begin{aligned}
0 = e \cdot \int_{\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}} \operatorname{div}(\Sigma_\varepsilon) \;\; &= \;\; e \cdot \left(\int_{\partial\Omega} \Sigma_\varepsilon n + \int_{\hat{\gamma}_\varepsilon} \Sigma_\varepsilon n - \int_{\gamma^*} \Sigma_\varepsilon n \right) \\
&= \;\; e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n - e \cdot \int_{\gamma^*} \Sigma_\varepsilon n \ . \quad\quad (3.28)
\end{aligned}
$$

which provides the result.

The shape derivative of the total potential energy, namely (3.26) or (3.27), 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

$$
G_\varepsilon = -\alpha \dot{\mathfrak{J}}_{\Omega_\varepsilon} = \alpha e \cdot \int_{\gamma^*} \Sigma_\varepsilon n = \alpha e \cdot \left(\lim_{\rho \to 0} \int_{\partial B_\rho^*} \Sigma_\varepsilon n \right) = \alpha e \cdot \int_{\partial\Omega} \Sigma_\varepsilon n \ , \quad (3.29)
$$

where B_ρ^* is any ball of radius $\rho > 0$ centered at the crack tip x^* (see fig. 4) 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), see also Destuynder and Djaoua (1981)).
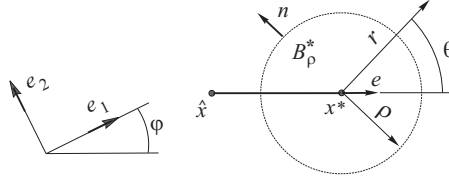

Figure 4: Polar coordinate system (r, θ).

It turns out that (3.29) 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.,

$$
g_\varepsilon^* = \lim_{\rho \to 0} \int_{\partial B_\rho^*} \Sigma_\varepsilon n \quad\quad \text{and} \quad\quad \dot{\mathfrak{J}}_{\Omega_\varepsilon} = -g_\varepsilon^* \cdot e \ . \quad\quad (3.30)
$$

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

13

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 (3.3) and (3.30) the topological derivative is introduced as

$$\texttt{TOPOLOGICAL DERIVATIVE} \qquad D_T\psi = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}g_\varepsilon^*\cdot e. \qquad (3.31)$$

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

$$\texttt{TOPOLOGICAL GRADIENT} \qquad G_T\psi = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}g_\varepsilon^*. \qquad (3.32)$$

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 SIFs 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 SIFs 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.

Their computation is the object of a extensive literature (see e.g. the handbooks of Sih (1973) or Tada et al. (2000)), which is justified by their crucial role in many model of crack evolution based either on the "maximisation of the dissipation" at the crack tip, or on the "$K_{\mathrm{II}} = 0$" evolution law.

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. 4) are considered. In particular, the displacement is written as

$$u_\varepsilon = u_\varepsilon^r(r,\theta)e_r + u_\varepsilon^\theta(r,\theta)e_\theta \ , \qquad (3.33)$$

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

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\left(3-\nu-(1+\nu)\cos\theta\right)\cos(\theta/2)\,, \quad (3.34)$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(3-\nu-(1+\nu)\cos\theta)\sin(\theta/2)\,, (3.35)$$

- for the mode II

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\left(3\nu-1+3(1+\nu)\cos\theta\right)\sin(\theta/2)\,, (3.36)$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}\left(5+\nu-3(1+\nu)\cos\theta\right)\cos(\theta/2) (3.37)$$

where $K_{\mathrm{I}}, K_{\mathrm{II}}$ are the SIFs 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 (3.30) can be taken arbitrarily close to the crack tip, and hence expressions (3.34)-(3.37) 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:

$$f(\varepsilon) = \pi\varepsilon^2 \tag{3.38}$$

in such a way that, by letting $\varepsilon \to 0$, the expressions (3.31) of the topological derivative and (3.32) of the topological gradient becomes

$$D_T\psi(u,e) = -\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) \quad \text{and} \quad G_T\psi(u,e) = -\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right)e\,, \tag{3.39}$$

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

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2\frac{\alpha}{4E}\left(K_{\mathrm{I}}^2+K_{\mathrm{II}}^2\right) + o(\varepsilon^2)\,. \tag{3.40}$$

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

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)\left(3-4\nu-\cos\theta\right)\cos(\theta/2)\,, \quad (3.41)$$

$$u_\varepsilon^\theta(r,\theta) = -\frac{K_{\mathrm{I}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)(3-4\nu-\cos\theta)\sin(\theta/2)\,, (3.42)$$

15

- for the mode II

$$u_\varepsilon^r(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)(4\nu-1+3\cos\theta)\sin(\theta/2) , \quad (3.43)$$

$$u_\varepsilon^\theta(r,\theta) = \frac{K_{\mathrm{II}}(u,e)}{E}\sqrt{\frac{r\varepsilon}{2}}(1+\nu)(4\nu-5+3\cos\theta)\cos(\theta/2) , \quad (3.44)$$

where $K_{\mathrm{I}}, K_{\mathrm{II}}$ are the SIFs 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 (3.31) and (3.32), that is

$$D_T\psi(u,e) = -\alpha\frac{1-\nu^2}{4E}\left(K_{\mathrm{I}}^2 + K_{\mathrm{II}}^2\right) \quad \text{and} \quad G_T\psi(u,e) = D_T\psi(u,e)e . \quad (3.45)$$

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

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2\alpha\frac{1-\nu^2}{4E}\left(K_{\mathrm{I}}^2 + K_{\mathrm{II}}^2\right) + o(\varepsilon^2) . \quad (3.46)$$

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 (3.39) and (3.45)) 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 (3.39) or (3.45) 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 (2.10) 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, (3.39) and (3.45) 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

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

$$(4.1)$$

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

16

The introduction of a precise notion of derivation for crack nucleation is also justified , since from the observation that the sole Griffith's critical relation:

$$G_\varepsilon = 2\pi\varepsilon\frac{K_{\text{I}}^2 + K_{\text{II}}^2}{E} = G_{crit} \tag{4.2}$$

where G_{crit} is a material dependent crack growth threshold would imply that the critical K_{I} and K_{II} are of the order of $1/\sqrt{\varepsilon}$, and hence would be unbounded (i.e., unphysical) as $\varepsilon \to 0$.

Let us remark that criterion (4.1) is only apparently based on a double minimization, and will eventually result in a sole minimization in x, since the optimal crack direction will be shown to obey a universal property of homogeneous linear elastic materials. It will be shown in the following two sections that the nucleation criterion only amounts to the minimization of the scalar field $D_T\psi(x, e(\varphi^\star))$ over $x \in \Omega$, as soon as the law providing optimal fracture direction (i.e., the angle $\varphi^\star$) is known.

It can be observed that the nucleation optimality criterion (4.1) is, by (3.3) and (3.38), equivalent to the maximization of $G_\varepsilon/\varepsilon$, where G_ε is the Griffith's energy release rate of a crack of length ε (this is sometimes called the Irwin's criterion). However while the latter criterion appears as a postulate (and is often referred to as a *principle*) in the classical literature on brittle fracture (see e.g. Irwin (1958); Cherepanov (1979); Lawn (1993); Lemaitre and Chaboche (1988)), it is here given a precise mathematical meaning. Moreover, it should be precised that while the maximal dissipation principle is sometimes used to predict crack evolution, by providing a method for finding the optimal direction e (see e.g. the book by Lemaitre and Chaboche (1988)), it is not specifically dedicated for crack nucleation predictions. Let us also finally remark that such a criterion, possibly combined with other methods, may provide a useful tool for numerical simulation of brittle crack quasi-static evolution.

In the following section, a geometric property for linear elastic cracked bodies will be proved.

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

$$K_{\text{I}} = \sigma(u)e^\perp \cdot e^\perp \qquad \text{and} \qquad K_{\text{II}} = \sigma(u)e \cdot e^\perp , \tag{4.3}$$

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

- for plane stress, as

$$D_T\psi = -\frac{1}{2E}\left[(\sigma(u)e^\perp \cdot e^\perp)^2 + (\sigma(u)e \cdot e^\perp)^2\right] , \tag{4.4}$$

- and for plane strain, as

$$D_T \psi = -\frac{1-\nu^2}{2E} \left[(\sigma(u)e^\perp \cdot e^\perp)^2 + (\sigma(u)e \cdot e^\perp)^2 \right] . \qquad (4.5)$$

In any of the two cases, the crack will, according to the above criterion (4.1), nucleate in a direction that minimizes the topological derivative. Hence, by writing

$$e = (\cos\varphi, \sin\varphi) \qquad \text{and} \qquad e^\perp = (-\sin\varphi, \cos\varphi) , \qquad (4.6)$$

where φ denotes the angle between the crack direction e and the local basis $\{e_1, e_2\}$ located at x (cf. Fig. 4), it suffices to find $\varphi^\star$ such that

$$\varphi^\star := \arg \left\{ \max_{0 \le \theta < 2\pi} \left[\sigma_{11}^2 + 2\sigma_{12}^2 + \sigma_{22}^2 + (\sigma_{22}^2 - \sigma_{11}^2)\cos(2\theta) - 2\sigma_{12}(\sigma_{11} + \sigma_{22})\sin(2\theta) \right] \right\} , \qquad (4.7)$$

which results in

$$\varphi^\star = \pm\frac{1}{2} \arccos \left(\pm\sqrt{\frac{(\sigma_{11} - \sigma_{22})^2}{(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}^2}} \right) \qquad (4.8)$$

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 *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 $K_{\text{II}} = 0$ nucleation criterion, instead of being simply postulated, can now be proved.

Proposition 5 ($K_{\text{II}} = 0$ nucleation criterion). *In homogeneous LEFM, the $K_{\text{II}} = 0$ crack nucleation criterion satisfies the property of minimal topological derivative, i.e., of maximal decrease of the total potential energy (2.10).*

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 (4.8) 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 $\varphi^\star = \pi/2$.

The *Local Symmetry Principle* is called $K_{\text{II}} = 0$ criterion because it means that locally the crack lips are in pure mode I, in the sense that the principal tractions apply on their faces. Strictly speaking, the above law holds for infinitesimal

cracks, whereas for cracks of finite length, other physical mechanisms should be taken into account (see e.g. Fischer and Göldner (1981); Bourdin et al. (2008)). Let us also mention that, unless the presence of impurities, brittle crack initiation in the sense of Griffith always implies cracks of finite lengh, as discussed by Bourdin et al. (2008) or Chambolle et al. (2008b), and hence at nucleation points, no infinitesimal crack will ever appear. This latter property will appear within our setting in section 5.

Moreover, Proposition 5 also contributes to the debate between the validity of Irwin's maximal dissipation criterion versus *Local Symmetry Principle*. In fact, Proposition 5 states that relying on Irwin's principle, a precise notion of nucleation is introduced via the topological derivative, whose minimal value coincide with the $K_{\mathrm{II}} = 0$ criterion and the principle of maximal traction.

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_{I} and K_{II} are given by (cf. Beghinia et al. (1999))

$$
\begin{pmatrix} K_{\mathrm{I}} \\ K_{\mathrm{II}} \end{pmatrix} = \begin{pmatrix} F_{\mathrm{I}}^{S} & F_{\mathrm{I}}^{T} \\ F_{\mathrm{II}}^{S} & F_{\mathrm{II}}^{T} \end{pmatrix} \begin{pmatrix} \sigma(u)e^{\perp} \cdot e^{\perp} \\ \sigma(u)e \cdot e^{\perp} \end{pmatrix} ,
\tag{4.9}
$$

where coefficients $F_{\mathrm{I}}^{S}, F_{\mathrm{I}}^{T}$ and $F_{\mathrm{II}}^{S}, F_{\mathrm{II}}^{T}$ 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

$$
\begin{aligned}
D_T \psi = & - \frac{1}{4E} \big[(F_{\mathrm{I}}^{S}\sigma(u)e^{\perp} \cdot e^{\perp} + F_{\mathrm{I}}^{T}\sigma(u)e \cdot e^{\perp})^2 \\
& + (F_{\mathrm{II}}^{S}\sigma(u)e^{\perp} \cdot e^{\perp} + F_{\mathrm{II}}^{T}\sigma(u)e \cdot e^{\perp})^2 \big] ,
\end{aligned}
$$

- and for plane strain, as

$$
\begin{aligned}
D_T \psi = & - \frac{1-\nu^2}{4E} \big[(F_{\mathrm{I}}^{S}\sigma(u)e^{\perp} \cdot e^{\perp} + F_{\mathrm{I}}^{T}\sigma(u)e \cdot e^{\perp})^2 \\
& + (F_{\mathrm{II}}^{S}\sigma(u)e^{\perp} \cdot e^{\perp} + F_{\mathrm{II}}^{T}\sigma(u)e \cdot e^{\perp})^2 \big] .
\end{aligned}
$$

In this case, there are no close representation for the SIFs K_{I} and K_{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.

4.3. Case 3: kinking

The case of kinking can in principle be addressed by our method, since approximation formulaes such as (4.9) have been derived by Amestoy and Leblond (1992) for small kinking angles. Concerning crack evolution in time including

kinking, and a discussion on time-continuity of cracks, we refer to Chambolle et al. (2008a, 2009).

It should also be noted that for a pre-existing crack, the evaluation of the SIFs is strongly dependent of the crack and body geometry, and hence for kinking analyses, we refer to Amestoy and Leblond (1992).

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

$$\Xi(\Omega_\varepsilon) = \psi(\Omega_\varepsilon) + C(\gamma_\varepsilon) \, , \tag{5.1}$$

with

$$C(\gamma_\varepsilon) = \int_{\gamma_\varepsilon} \kappa(\varepsilon) \, , \tag{5.2}$$

whose simplest expression is taken as

$$C(\gamma_\varepsilon) = \tilde{\kappa}\varepsilon \, , \tag{5.3}$$

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 (2.9).

From (5.3) it follows that the derivative w.r.t. ε of $C(\gamma_\varepsilon)$ is given by

$$\dot{C}(\gamma_\varepsilon) = \tilde{\kappa} > 0 \, . \tag{5.4}$$

whereby from (3.40) or (3.46) and (5.4) it results that $\Xi(\Omega_\varepsilon)$ admits the following total derivative w.r.t. ε:

$$\dot{\Xi}(\Omega_\varepsilon) = \tilde{\kappa} + O(\varepsilon) \, , \tag{5.5}$$

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

$$D_T\Xi = \lim_{\varepsilon \to 0} \left(\frac{1}{f'_\Xi(\varepsilon)} \dot{\Xi}(\Omega_\varepsilon) \right) = \tilde{\kappa} > 0 \, . \tag{5.6}$$

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 (4.1) as applied to (5.1) and (5.3), there will be no infinitesimal crack nucleation.*

20

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 explicitly bounded from below. In fact, the topological asymptotic expansion of the shape functional (5.1) reads

$$\Xi(\Omega_\varepsilon) = \Xi(\Omega) + \varepsilon\tilde{\kappa} + \pi\varepsilon^2 D_T\psi + o(\varepsilon^2) . \qquad (5.7)$$

where $D_T\psi$ can be obtained from (3.40) and (3.46) 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.

- for plane stress

$$\varepsilon^\star > \frac{2\tilde{\kappa}E}{\pi K_{\mathrm{I}}^2} ; \qquad (5.8)$$

- for plane strain

$$\varepsilon^\star > \frac{2\tilde{\kappa}E}{\pi(1-\nu^2)K_{\mathrm{I}}^2} ; \qquad (5.9)$$

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 (2.9) and given its asymptotic expression in terms of the small crack length ε, the

21

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.

References

Allaire, G., de Gournay, F., Jouve, F., Toader, A.-M., 2005. Structural optimization using topological and shape sensitivity via a level set method. Control and Cybernetics 34 (1), 59–80.

Allaire, G., Jouve, F., Toader, A.-M., 2004. Structural optimization using sensitivity analysis and a level-set method. Journal of Computational Physics 194 (1), 363–393.

Allaire, G., Jouve, F., Van Goethem, N., 2007. A level set method for the numerical simulation of damage evolution. In: ICIAM Proceedings. Zürich, Switzerland.

Amestoy, M., Leblond, J.-B., 1992. Crack paths in plane situations.ii.detailed form of the expansion of the stress intensity factors. Int. J. Solids Struct. 29 (4), 465–501.

Ammari, H., Kang, H., 2004. Reconstruction of small inhomogeneities from boundary measurements. Lectures Notes in Mathematics vol. 1846. Springer-Verlag, Berlin.

Amstutz, S., Andrä, H., 2006. A new algorithm for topology optimization using a level-set method. Journal of Computational Physics 216 (2), 573–588.

Amstutz, S., Horchani, I., Masmoudi, M., 2005. Crack detection by the topological gradient method. Control and Cybernetics 34 (1), 81–101.

Auroux, D., Masmoudi, M., Belaid, L., 2007. Image restoration and classification by topological asymptotic expansion. In: Variational formulations in mechanics: theory and applications. Barcelona, Spain.

Barenblatt, G., Cherepanov, G., 1961. On brittle cracks under longitudinal shear. PMM 25, 1110–1119.

Beghinia, M., Bertinia, L., Fontanari, V., 1999. Stress intensity factors for an inclined edge crack in a semiplane. Engineering Fracture Mechanics 62 (6), 607–613.

Belaid, L., Jaoua, M., Masmoudi, M., Siala, L., 2008. Application of the topological gradient to image restoration and edge detection. Engineering Analysis with Boundary Element 32 (11), 891–899.

Bourdin, B., Francfort, G., Marigo, J.-J., 2000. Numerical experiments in revisited brittle fracture. Journal of the Mechancis and Physics of Solids 48 (4), 797–826.

Bourdin, B., Francfort, G., Marigo, J.-J., 2008. The Variational Approach to Fracture. Springer-Verlag.

Bourdin, B., Larsen, C. J., Richardson, C., 2009. A time-discrete model for dynamic fracture based on crack regularization. Tech. rep.

Burger, M., Hackl, B., Ring, W., 2004. Incorporating topological derivatives into level set methods. Journal of Computational Physics 194 (1), 344–362.

Céa, J., Garreau, S., Guillaume, P., Masmoudi, M., 2000. The shape and topological optimizations connection. Computer Methods in Applied Mechanics and Engineering 188 (4), 713–726.

Chambolle, A., Francfort, G., Marigo, J.-J., 2008a. Revisiting energy release rates in brittle fracture. Tech. Rep. 646, Centre de Mathématiques Appliquées.

Chambolle, A., Francfort, G., Marigo, J.-J., 2009. When and how do crack propagate? Tech. Rep. 654, Centre de Mathématiques Appliquées.

Chambolle, A., Giacomini, A., Ponsiglione, M., 2008b. Crack initiation in brittle materials. Arch. Rational Mech. Anal. 188, 309–349.

Cherepanov, G., 1979. Mechanics of Brittle Fracture. McGraw Hill, New York.

Destuynder, P., Djaoua, M., 1981. Sur une interprétation mathématique de lintégrale de rice en théorie de la rupture fragile. Mathematical Methods in Applied Sciences 3, 70–87.

Erdogan, F., Sih, G., 1963. On the crack extension in plates under plane loading and transverse shear. J. Bas. Engng., Trans. ASME, Ser. D 85, 519527.

Eshelby, J., 1975. The elastic energy-momentum tensor. Journal of Elasticity 5 (3-4), 321–335.

Feijóo, G., 2004. A new method in inverse scattering based on the topological derivative. Inverse Problems 20 (6), 1819–1840.

Feijóo, R., Padra, C., Saliba, R., Taroco, E., Vénere, M., Marcelo, J., 2000. Shape sensitivity analysis for energy release rate evaluation and its application to the study of three-dimensional cracked bodies. Computer Methods in Applied Mechanics and Engineering 188 (4), 649–664.

Fischer, K.-F., Göldner, H., 1981. On the formulation of a principal strain criterion in crack fracture mechanics. International Journal of Fracture 17 (1), R3–R6.

Francfort, G., Marigo, J.-J., 1998. Revisiting brittle fracture as an energy minimization problem. Journal of the Mechanics and Physics of Solids 46 (8), 1319–1342.

Griffiths, A., 1921. The phenomena of rupture and flow in solids. Philosofical Transaction of the Royal Society. 221, 163–198.

Grisvard, P., 1989. Singularités en elasticité. Archives for Rational Mechanics and Analysis 107, 157–180.

Gurtin, M., 1981. An introduction to continuum mechanics. Mathematics in Science and Engineering vol. 158. Academic Press, New York.

Gurtin, M., 2000. Configurational forces as basic concept of continuum physics. Applied Mathematical Sciences vol. 137. Springer-Verlag, New York.

Hakim, V., Karma, A., 2008. Laws of crack motion and phase-field models of fracture. Journal of the Mechanics and Physics of Solids 57 (2), 342–368.

Hintermüller, M., 2005. Fast level set based algorithms using shape and topological sensitivity. Control and Cybernetics 34 (1), 305–324.

Irwin, G., 1958. Fracture. In Handbuch der Physik 6, 551–590.

Knees, D., Mielke, A., Zanini, C., 2002. On the inviscid limit of a model for crack propagation. Mathematical Models and Methods in Applied Sciences 18 (9), 1529–1568.

Larrabide, I., Feijóo, R., Novotny, A., Taroco, E., 2008. Topological derivative: a tool for image processing. Computers & Structures 86 (13-14), 1386–1403.

Lawn, B., 1993. Fracture of Brittle Solids 2nd ed. Cambridge University Press, Cambridge, England.

Lee, S., Kwak, B., 2008. Smooth boundary topology optimization for eigenvalue performance and its application to the design of a flexural stage. Enginnering Optmization 40 (3), 271–285.

Lemaitre, J., Chaboche, J.-L., 1988. Mecanique des materiaux solides. Paris Dunod, Paris.

Masmoudi, M., Pommier, J., Samet, B., 2005. The topological asymptotic expansion for the Maxwell equations and some applications. Inverse Problems 21 (2), 547–564.

Moës, N., Gravouil, A., Belytschko, T., 2002a. Non-planar 3d crack growth by the extended finite element and level sets-part i: Mechanical model. International Journal for Numerical Methods in Engineering 53 (11), 2549–2568.

Moës, N., Gravouil, A., Belytschko, T., 2002b. Non-planar 3d crack growth by the extended finite element and level sets-part ii: Level set update. International Journal for Numerical Methods in Engineering 53 (11), 2569–2586.

Nazarov, S., Sokołowski, J., 2003. Asymptotic analysis of shape functionals. Journal de Mathématiques Pures et Appliquées 82 (2), 125–196.

Novotny, A., Feijóo, R., Padra, C., Taroco, E., 2003. Topological sensitivity analysis. Computer Methods in Applied Mechanics and Engineering 192 (7-8), 803–829.

Novotny, A., Feijóo, R., Padra, C., Taroco, E., 2005. Topological derivative for linear elastic plate bending problems. Control and Cybernetics 34 (1), 339–361.

Novotny, A., Feijóo, R., Taroco, E., Padra, C., 2007. Topological sensitivity analysis for three-dimensional linear elasticity problem. Computer Methods in Applied Mechanics and Engineering 196 (41-44), 4354–4364.

Rice, J., 1968. A path independent integral and the approximate analysis of strain concentration by notches and cracks. Journal of Applied Mechenics 35, 145–153.

Sih, G. C., 1973. Handbook of Stress Intensity Factors. Institute of Fracture and Solid Mechanics. Lehigh University, Bethlehem, Pennsylvania.

Sokołowski, J., Żochowski, A., 1999. On the topological derivatives in shape optmization. SIAM Journal on Control and Optimization 37 (4), 1251–1272.

Sokołowski, J., Żochowski, A., 2001. Topological derivatives of shape functionals for elasticity systems. Mechanics of Structures and Machines 29 (3), 333–351.

Sokołowski, J., Zolésio, J.-P., 1992. Introduction to shape optimization - shape sensitivity analysis. Springer-Verlag, New York.

Song, J.-H., Wang, H., Belytschko, T., 2008. A comparative study on finite element methods for dynamic fracture. Comput. Mech. 42, 23–250.

Tada, H., Paris, P., Irwin, G., 2000. The stress analysis of cracks handbook. ASME Press, New York.