

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 (LEFM). In particular, the topological asymptotic expansion of the total potential energy together with a Griffith-type energy of an elastic cracked body is calculated. As main result, 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.

1. INTRODUCTION

The theory of brittle fracture takes its origin in the work of Griffith [38], later pursued by the key theoretical contributions by Cherepanov [27], Erdogan [29], Irwin [46] and Rice [60] – among others. In the 80ies several contributions (cf., e.g., [4, 5, 52]) paved the way for the numerical simulation of crack evolution (cf., e.g., [14, 20, 54, 55]). Most of these approaches have proved a long time ago their physical validation and shown useful engineering applications. However, only a few of them have been fully mathematically justified.

About 15 years ago Francfort and Marigo [34] introduced a mathematical approach to brittle fracture called “variational brittle fracture”, which remains nowadays a subject of intensive research [21, 26]. One of their main contribution was to avoid the specification of a known crack path for crack predictions, while focussing on solutions obtained by a global minimization approach in a quasi-static setting. However, according to Miehe et al. [48], one drawback of global solutions is to predict underestimated crack initiation times. Today, their original approach is also being extended to dynamic crack growth [22], while local approaches are also addressed from a numerical viewpoint [2]. Discussions on the question of time-continuity of crack paths as related to kinking criteria can also be found in the recent literature [25].

In general, analysis of crack propagation considers an already cracked body. 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, but this criterion failed to predict general cracked bodies where the loads are not aligned with the crack. In order to generalize this observation, the concept of stress intensity factors (SIF) [64] as a measure of stress in the crack process zones appeared useful and soon reached consensus. Later, instead of relying on a simple critical SIF criterion, a local criterion based on the so-called *strain-energy density functions* was suggested [61], while other works [46, 60] proposed local crack growth principles based on the notion of *maximal dissipation* at the crack tip. On the other hand, relying on symmetry arguments, Barenblatt and Cherepanov [16] proposed yet another local criterion based on the principle that the crack grows with *vanishing (shearing) mode II*, also known as *the principle of local symmetry* (see also [37]). However, all these local methods are not easily tractable in the applications since relying on the permanent re-evaluation of the SIF for every new cracked body configuration. Moreover, as shown by Amestoy and Leblond [5], these various coexisting criteria are not equivalent from a physical viewpoint, and therefore the continued interest in mathematical approaches is justified [42].

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,

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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 length as well as for infinitesimal cracks, i.e., for nucleation. From a mathematical viewpoint, Chambolle et al. [26] have derived several results relating crack initiation to a local measure of singularity, that is, to the presence, or not, of defects in the elastic body. In particular, they have proved that in the absence of defects, brittle fracture can only occur brutally, that is, with a critical minimal crack length.

In this paper, we propose a general exact analytical expression for crack nucleation sensitivity analysis. Here, the sensitivity is a scalar field which measures how the elastic energy (or, in general, an appropriate 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 [24,62] 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 [62] 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 [11, 36, 56]. Its use in the context of topology optimization of load bearing structures [1–3, 12, 23, 51, 58, 59], inverse problems [13, 31, 44, 53] and image processing [15, 18, 43, 45, 49] are among the main applications of this analytical tool. Concerning the theoretical development associated to the powerful methods derived from the asymptotic analysis of PDE solutions, the reader may refer for instance to [8–10]. See also [6,7,47] for applications of these ideas to inverse problems.

As main results of this paper, we propose the following:

- (1) a crack nucleation criterion based on the topological derivative
- (2) a criterion for determining the direction of crack growth based on the topological gradient
- (3) a nucleation result linking the maximal dissipation, vanishing mode II, and maximal stress criteria (which do not classically coincide)
- (4) an alternative proof of the brutal crack nucleation in Griffith's setting.

Let us emphasize that all these results cannot be claimed new. Nevertheless, to our knowledge the original contribution of this paper is to establish an *axiomatic approach* to address 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 here an a priori requirement.

Moreover, with a view to practical application of this theory, let us remark that the *intrinsic local* notion of the topological derivative as a nucleation criterion is a tool which can eventually be used to perform numerical simulation of crack nucleation and growth. We refer to [2] for a method which could easily be coupled with the concepts as presented in this paper.

The paper is organized as follows. The mechanical model associated to plane stress and plane strain linear elasticity is described in section 2. In section 3 we 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 in [57]. In section 3.1 we extend our theory for cracked bodies. Following the original ideas presented in [32], 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 4, where we derive closed formulas for the crack nucleation sensitivity

analysis. Section 5 is dedicated to the interpretation of the obtained topological derivative and gradient in terms of optimization properties. In section 6, another energy criterion, including surface contributions, is analysed within our method. Finally, some concluding remarks are made in section 7.

2. THE MECHANICAL MODEL

Let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$ with smooth boundary $\partial\Omega = \Gamma_N \cup \Gamma_D$ ($\Gamma_N \cap \Gamma_D = \emptyset$), 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^* , 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

$$\nabla^s \xi := \frac{1}{2} (\nabla \xi + \nabla \xi^T) \quad \text{and} \quad \sigma(\xi) = \mathbb{C} \nabla^s \xi, \quad (1)$$

respectively, where ξ represents an admissible displacement field, $(\nabla \xi)_{ij} = \partial_j \xi_i$, $(\nabla \xi^T)_{ij} = \partial_i \xi_j$. In addition, \mathbb{C} is the (symmetric) isotropic elasticity tensor given by

$$\mathbb{C} = 2\mu \mathbb{I} + \lambda (I \otimes I), \quad (2)$$

where μ and λ are the Lamé coefficients, that is

$$\mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \quad \text{and} \quad \lambda = \lambda^* = \frac{\nu E}{1-\nu^2}, \quad (3)$$

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 (see Fig. 1), which is in equilibrium if the following variational problem holds: find the displacement field $u \in \mathcal{U}$, such that

$$\int_{\Omega} \sigma(u) \cdot \nabla^s \eta = \int_{\Omega} b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \quad \forall \eta \in \mathcal{V}, \quad (4)$$

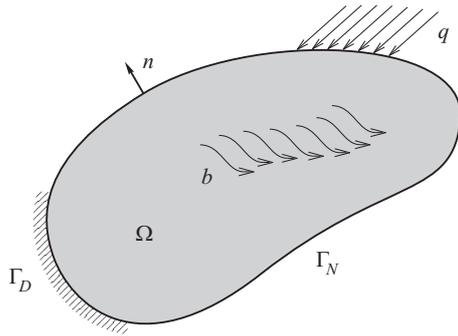
where $\sigma(u) = \mathbb{C} \nabla^s u$, \mathcal{U} is the set of admissible displacements and \mathcal{V} the space of admissible variations, which are respectively defined, for $b \in L^2(\Omega)$ and $h, q \in L^2(\partial\Omega)$, as

$$\mathcal{U} := \left\{ u \in H^1(\Omega) : u|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V} := \left\{ \eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0 \right\}. \quad (5)$$

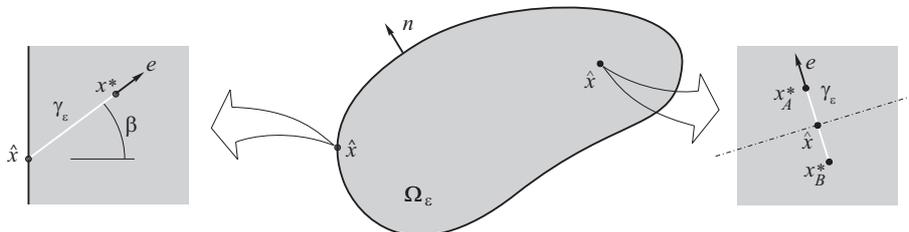
The above variational problem has a unique solution and corresponds to the weak formulation of the momentum conservation law with appropriate boundary conditions:

$$\begin{cases} -\operatorname{div}(\sigma(u)) = b & \text{in } \Omega \\ \sigma(u) = \mathbb{C} \nabla^s u \\ u = h & \text{on } \Gamma_D \\ \sigma(u)n = q & \text{on } \Gamma_N \end{cases}, \quad (6)$$

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 length 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 we will consider cracks which are segments $\gamma_\varepsilon = [x_A^*; x_B^*] \subset \Omega$, where x_A^* and x_B^* are the crack tips. In this case, since the size ε of the crack is a small parameter, which tends to zero, the stress distribution around the crack extremities x_A^* and x_B^* is 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 an angle β defined with respect to the direction of n on $\partial\Omega$. In general, we will consider cracks which are segments $\gamma_\varepsilon = [\hat{x}; x^*] \subset \overline{\Omega}$, 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

$$\int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \eta = \int_{\Omega_\varepsilon} b \cdot \eta + \int_{\Gamma_N} q \cdot \eta \quad \forall \eta \in \mathcal{V}_\varepsilon, \quad (7)$$

where $\sigma(u_\varepsilon) = \mathbb{C} \nabla^s u_\varepsilon$, \mathcal{U}_ε is the set of admissible displacements and \mathcal{V}_ε 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

$$\mathcal{U}_\varepsilon := \left\{ u_\varepsilon \in H^1(\Omega_\varepsilon) : u_\varepsilon|_{\Gamma_D} = h \right\} \quad \text{and} \quad \mathcal{V}_\varepsilon := \left\{ \eta \in H^1(\Omega_\varepsilon) : \eta|_{\Gamma_D} = 0 \right\}. \quad (8)$$

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:

$$\left\{ \begin{array}{ll} -\operatorname{div}(\sigma(u_\varepsilon)) = b & \text{in } \Omega_\varepsilon \\ \sigma(u_\varepsilon) = \mathbb{C} \nabla^s u_\varepsilon & \\ u_\varepsilon = h & \text{on } \Gamma_D \\ \sigma(u_\varepsilon)n = q & \text{on } \Gamma_N \\ \sigma(u_\varepsilon)n = 0 & \text{on } \gamma_\varepsilon \end{array} \right. . \quad (9)$$

Let us remark that, since the perturbed domain is non-Lipschitz, the solution of (9), as opposed that of to (6) does not belong to $H^2(\Omega_\varepsilon)$. In particular the stress is singular at the crack

tip, and the displacement jumps across γ_ε . Let us remark that the tip singularity is due to the inadequacy of the linear elastic model near the crack extremities. Moreover, the last condition in (9) amounts to neglect the dynamic effect of cohesive forces between the crack lips, but their inter-penetration (i.e., negative normal jump component of the displacement at the crack) is not prohibited in the above model. This latter classical drawback of linear fracture mechanics will not be discussed any further in the sequel.

The solution to (9) is known to minimize

$$\mathfrak{J}_{\Omega_\varepsilon}(v) = \frac{1}{2} \int_{\Omega_\varepsilon} \sigma(v) \cdot \nabla^s v - \int_{\Omega_\varepsilon} b \cdot v - \int_{\Gamma_N} q \cdot v, \quad (10)$$

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 (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. Let us observe that for any crack, $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) \leq \mathfrak{J}_{\Omega_\varepsilon}(u) = \mathfrak{J}_\Omega(u)$, where the solution to the unperturbed problem u is a candidate with vanishing jump for the minimum problem (10). Therefore, 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 of a surface energy concentrated on the crack to take into account crack growth. Accordingly, the so-called Griffith's and Barenblatt's-type variational models are discussed in [21] with a view to determining crack initiation and path prediction.

In this paper, we show how the shape functional (10) can provide some relevant information as far as initiation of a single crack is concerned. In fact, the energy (10) is the simplest case addressed by our method. Surface energies can be added, and in general any refinement of (10) can be considered – provided it admits a topological derivative – within this sensitivity analysis setting. Two other ingredients are required in order to apply the present method: (i) the knowledge of the asymptotic expansion of the solution around the crack tip, and (ii) a shape derivative expression involving a divergence-free Eshelby-type tensor. One example of crack nucleation with Griffith's-type surface energy will be addressed in section 6.

Let us remark that the case of cracks with a non penetration condition on γ^* cannot be considered within this setting since the tip expansion of the solution is not known [35].

3. SHAPE AND TOPOLOGICAL DERIVATIVES

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

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f(\varepsilon) D_T \psi + o(f(\varepsilon)), \quad (11)$$

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 which depends on the asymptotic behavior of the problem under analysis, satisfying

$$\lim_{\varepsilon \rightarrow 0^+} f(\varepsilon) = 0, \quad (12)$$

where $o(f(\varepsilon))$ contains all terms of higher order in $f(\varepsilon)$.

Expression (11) 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. In general, expansion (11) cannot 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 [57], whereby the topological derivative is obtained as the limit

$$D_T \psi = \lim_{\varepsilon \rightarrow 0} \left(\frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\Omega_\varepsilon) \right). \quad (13)$$

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 [63] – with respect to the size ε of γ_ε . This term is classically termed the *shape derivative*. See also [19].

The advantage of definition (13) for the topological derivative is that the whole mathematical framework developed for the shape sensitivity analysis can be used as an intermediate step to calculate the topological derivative. This feature was shown in [57] for circular holes and it is now extended when the domain is perturbed by introducing a small crack.

In order to render this work as self-contained as possible, the remaining of this section is devoted to prove some classical results concerning shape sensitivity.

3.1. Shape sensitivity of 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 as the straight crack γ_ε grows, an appropriated shape change velocity field has to be defined. Thus, we consider an uncracked control volume ω^* with boundary γ^* such that $x^* \in \omega^*$. Then, we can define its cracked counterpart as $\omega_\varepsilon^* = \omega^* \setminus \gamma_\varepsilon$. Moreover let η^* denote a neighborhood of the crack tip x^* . From these elements, the following kinematically admissible *shape change velocity* sets are introduced

$$\mathcal{M} := \{V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega, V \cdot n = 0 \text{ in } \eta^* \cap \gamma_\varepsilon\} \quad (14)$$

$$\mathcal{M}_1 := \{V \in C^\infty(\Omega_\varepsilon) : V = 0 \text{ on } \partial\Omega, V = e \text{ in } \overline{\omega_\varepsilon^*}\} \quad (15)$$

$$\mathcal{M}_2 := \{V \in C^\infty(\Omega_\varepsilon) : V = -e \text{ on } \partial\Omega, V = 0 \text{ in } \overline{\omega_\varepsilon^*}\}, \quad (16)$$

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 .

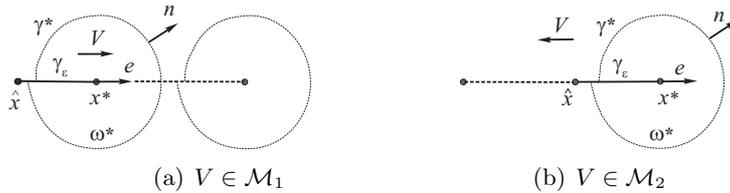


FIGURE 3. Shape change velocity field.

3.2. Rice invariance property and shape derivative expressions. The concept of energy release rate [38] 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 [32] a systematic methodology was presented in order to obtain the expression of energy release rate in cracked bodies based on shape sensitivity analysis.

Let us restate the equivalence between the concept of energy release rate and the shape sensitivity analysis of the functional

$$\psi(\Omega_\varepsilon) := \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - \int_{\Omega_\varepsilon} b \cdot u_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon, \quad (17)$$

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 [40] or, for analogies of this type in the context of shape sensitivity analysis, [63]).

The following notation is introduced:

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) := \left\langle \frac{\partial}{\partial \Omega_\varepsilon} \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon), V \right\rangle = \frac{d}{d\varepsilon} \mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon), \quad (18)$$

according to the definition of the shape change velocity sets \mathcal{M}_1 (15) or \mathcal{M}_2 (16) 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 (17). Then, its derivative with respect to the small parameter ε can be written as*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega_\varepsilon} \Sigma(u_\varepsilon)n \cdot V, \quad (19)$$

where V is any shape change velocity field belonging to \mathcal{M} , while Σ is a generalization of the classical Eshelby momentum-energy tensor [30, 41], given by

$$\Sigma(u_\varepsilon) := \frac{1}{2}(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)I - \nabla u_\varepsilon^T \sigma(u_\varepsilon). \quad (20)$$

Proof. Let us calculate the shape derivative of the functional $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ using the following version for the Reynolds' Transport Theorem [40, 63],

$$\begin{aligned} \dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2} \int_{\Omega_\varepsilon} (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)' + \frac{1}{2} \int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)V \cdot n - \int_{\Omega_\varepsilon} b \cdot u'_\varepsilon \\ &\quad - \int_{\partial\Omega_\varepsilon} (b \cdot u_\varepsilon)V \cdot n - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot u_\varepsilon \operatorname{div}_{\partial\Omega}(V), \end{aligned} \quad (21)$$

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 and the total derivatives with respect to ε , i.e.,

$$u'_\varepsilon := \partial_\varepsilon u_\varepsilon \quad \text{and} \quad \dot{u}_\varepsilon := u'_\varepsilon + \nabla u_\varepsilon V.$$

Let us observe that the last term on the RHS of (21) vanishes by the definition of the velocity field. Moreover, 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 [39] that the solution u_ε can be represented by 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 (21) is, because of that singular term, not well-defined at the crack tip, unless $V \cdot n$ vanishes, which is indeed assumed. Next, by using the concept of material derivatives of spatial fields we find that the first term of the above RHS integral can be written as

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

where the last term inside the parenthesis, as integrated over Ω_ε , is given a meaning by integration by parts 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

$$\begin{aligned} \dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2} \int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)V \cdot n - \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V) \\ &\quad + \int_{\Omega_\varepsilon} b \cdot \nabla u_\varepsilon V + \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} b \cdot \dot{u}_\varepsilon - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon. \end{aligned} \quad (22)$$

Since $\dot{u}_\varepsilon \in \mathcal{V}_\varepsilon$, the equilibrium equation (7) implies that the last three terms of (22) vanish, and hence

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\partial\Omega_\varepsilon} (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon - 2b \cdot u_\varepsilon)V \cdot n - \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V) + \int_{\Omega_\varepsilon} b \cdot \nabla u_\varepsilon V. \quad (23)$$

Eventually, using the tensor relation

$$\operatorname{div}(\sigma(u_\varepsilon)(\nabla u_\varepsilon V)) = \sigma(u_\varepsilon) \cdot \nabla^s(\nabla u_\varepsilon V) + \operatorname{div}(\sigma(u_\varepsilon)) \cdot \nabla u_\varepsilon V, \quad (24)$$

and the divergence theorem, expression (23) can be written as

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \Sigma(u_\varepsilon)n \cdot V + \int_{\Omega_\varepsilon} [\operatorname{div}(\sigma(u_\varepsilon)) + b] \cdot \nabla u_\varepsilon V, \quad (25)$$

and since the stress field $\sigma(u_\varepsilon)$ is in equilibrium, the proof of (19) simply results from (9). \square

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, instead of its boundary, is obtained.

Proposition 2 (Second form of the shape derivative). *Let $\mathfrak{J}_{\Omega_\varepsilon}(u_\varepsilon)$ be the functional defined by (17). Then, the derivative of the functional $\mathfrak{J}_{\Omega_\varepsilon}$ with respect to the small parameter ε is given by*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\Omega_\varepsilon} \Sigma(u_\varepsilon) \cdot \nabla V - \int_{\Omega_\varepsilon} \nabla b V \cdot u_\varepsilon, \quad (26)$$

where V is any shape change velocity field belonging to \mathcal{M} and Σ is given by (20).

Proof. Another version of Reynolds' Transport Theorem [40, 63] provides the identity

$$\begin{aligned} \dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2} \int_{\Omega_\varepsilon} [(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)' + (\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon) \operatorname{div}(V)] - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon \\ &\quad - \int_{\Omega_\varepsilon} [(b \cdot u_\varepsilon)' + (b \cdot u_\varepsilon) \operatorname{div}(V)] - \int_{\Gamma_N} q \cdot u_\varepsilon \operatorname{div}_{\partial\Omega}(V), \end{aligned} \quad (27)$$

Once again, the last term on the RHS of (27) vanishes by the definition of the velocity field. Next, by using the concept of material derivative of a spatial field [40, 63], we find that the first term of the above RHS integral can be written as

$$(\sigma(u_\varepsilon) \cdot \nabla^s u_\varepsilon)' = 2\sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - 2\nabla u_\varepsilon^T \sigma(u_\varepsilon) \cdot \nabla V, \quad (28)$$

which, substituted in (27) gives

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \Sigma(u_\varepsilon) \cdot \nabla V + \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla^s \dot{u}_\varepsilon - \int_{\Omega_\varepsilon} (b \cdot u_\varepsilon)' - \int_{\Gamma_N} q \cdot \dot{u}_\varepsilon, \quad (29)$$

Since $\dot{u}_\varepsilon \in \mathcal{V}_\varepsilon$, and with the equilibrium equation (7), the last three terms of (29) reduce to $-\int_{\Omega_\varepsilon} \dot{b} \cdot u_\varepsilon$, thereby proving the result. \square

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). *Provided the body force b is constant, the Eshelby tensor $\Sigma(u_\varepsilon)$ is a divergence-free tensor field away from the crack tip.*

Proof. By applying the divergence theorem to the right hand side of (26), we have

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega_\varepsilon} \Sigma(u_\varepsilon)n \cdot V - \int_{\Omega_\varepsilon} \operatorname{div}(\Sigma(u_\varepsilon)) \cdot V. \quad (30)$$

Since (19) and (26) hold for any velocity fields in \mathcal{M} , it results that

$$\int_{\Omega_\varepsilon} \operatorname{div}(\Sigma(u_\varepsilon)) \cdot V = 0 \quad \forall V \in \mathcal{M} \quad \Rightarrow \quad \operatorname{div}(\Sigma(u_\varepsilon)) = 0 \text{ a.e. in } \Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}. \quad (31)$$

\square

Proposition 4 (Rice integral). *Provided the body force b is constant, for any control volume ω^* containing the crack tip x^* with boundary γ^* , the shape derivative of the total potential energy for a variation in the direction e of a crack of length ε reads*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = e \cdot \int_{\partial\Omega} \Sigma(u_\varepsilon)n = e \cdot \int_{\gamma^*} \Sigma(u_\varepsilon)n, \quad (32)$$

where Σ is given by (20).

Proof. Let us define $\hat{\gamma}_\varepsilon = \gamma_\varepsilon \cap (\Omega \setminus \overline{\omega_\varepsilon^*})$. Since $\operatorname{div}(\Sigma(u_\varepsilon)) = 0$ in $\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}$ it results that the shape derivative of the total potential energy given by (26), after integrating by parts, becomes

$$\begin{aligned} \dot{\mathfrak{J}}_{\Omega_\varepsilon} &= \int_{\Omega_\varepsilon} \Sigma(u_\varepsilon) \cdot \nabla V = \int_{\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}} \Sigma(u_\varepsilon) \cdot \nabla V + \int_{\omega_\varepsilon^*} \Sigma(u_\varepsilon) \cdot \nabla V \\ &= \int_{\partial\Omega} \Sigma(u_\varepsilon)n \cdot V + \int_{\hat{\gamma}_\varepsilon} \Sigma(u_\varepsilon)n \cdot V - \int_{\gamma^*} \Sigma(u_\varepsilon)n \cdot V + \int_{\omega_\varepsilon^*} \Sigma(u_\varepsilon) \cdot \nabla V. \end{aligned} \quad (33)$$

Let us consider the velocity field $V \in \mathcal{M}_2$ given by (16) in the above result (33), which implies

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega} \Sigma(u_\varepsilon)n \cdot V + \int_{\hat{\gamma}_\varepsilon} \Sigma(u_\varepsilon)n \cdot V \quad \text{with } V \in \mathcal{M}_2. \quad (34)$$

Taking into account that $n \perp V$ on $\hat{\gamma}_\varepsilon$ and considering that $\sigma(u_\varepsilon)n = 0$ on $\hat{\gamma}_\varepsilon$, equation (34) becomes

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = \int_{\partial\Omega} \Sigma(u_\varepsilon)n \cdot V = -e \cdot \int_{\partial\Omega} \Sigma(u_\varepsilon)n \quad \text{with } V \in \mathcal{M}_2. \quad (35)$$

If, in turn, the velocity field $V \in \mathcal{M}_1$ given by (15) is inserted in (33), it results, by using the same arguments as above, that

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = - \int_{\gamma^*} \Sigma(u_\varepsilon)n \cdot V = -e \cdot \int_{\gamma^*} \Sigma(u_\varepsilon)n \quad \text{with } V \in \mathcal{M}_1. \quad (36)$$

On the other hand, by considering (31) and since $\partial(\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}) = \partial\Omega \cup \hat{\gamma}_\varepsilon \cup \gamma^*$, it can be shown that (35) and (36) are equivalents:

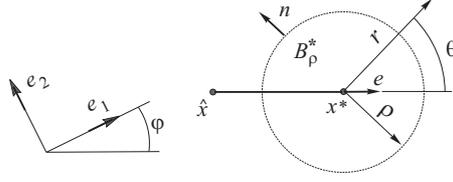
$$\begin{aligned} 0 &= e \cdot \int_{\Omega_\varepsilon \setminus \overline{\omega_\varepsilon^*}} \operatorname{div}(\Sigma(u_\varepsilon)) = e \cdot \left(\int_{\partial\Omega} \Sigma(u_\varepsilon)n + \int_{\hat{\gamma}_\varepsilon} \Sigma(u_\varepsilon)n - \int_{\gamma^*} \Sigma(u_\varepsilon)n \right) \\ &= e \cdot \int_{\partial\Omega} \Sigma(u_\varepsilon)n - e \cdot \int_{\gamma^*} \Sigma(u_\varepsilon)n, \end{aligned} \quad (37)$$

where the above result was obtained with help of the divergence theorem for second-order tensor fields and taking into account the fact that on $\hat{\gamma}_\varepsilon$ we have $n \cdot e = 0$ and $\sigma(u_\varepsilon)n = 0$, implying in $\Sigma(u_\varepsilon)n \cdot e = 0$ on $\hat{\gamma}_\varepsilon$. \square

The shape derivative of the total potential energy, namely (35) or (36), 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 of the energy release rate is independent of the value of V at the interior of the domain Ω_ε . In addition, since γ^* is an arbitrary curve around the crack tip x^* , the energy release rate due the crack growth can be written as

$$G_\varepsilon := -\alpha \dot{\mathfrak{J}}_{\Omega_\varepsilon} = \alpha e \cdot \int_{\partial\Omega} \Sigma(u_\varepsilon)n = \alpha e \cdot \int_{\gamma^*} \Sigma(u_\varepsilon)n = \alpha e \cdot \int_{\partial B_\rho^*} \Sigma(u_\varepsilon)n, \quad (38)$$

where B_ρ^* is the ball of radius $\rho \ll \varepsilon$ centered at the crack tip x^* (see Fig. 4) and α is the number of crack extremities ($\alpha = 1$ for $\hat{x} \in \partial\Omega$ and $\alpha = 2$ for $\hat{x} \in \Omega$). Let us mention that the energy release rate classically coincides with the Rices's integral [28, 60].

FIGURE 4. Polar coordinate system (r, θ) .

It turns out that (38) also provides the definition of the configurational force [41] denoted by g_ε^* as exerted at the crack tip x^* , and hence (38) enlightens the following relation between force, velocity and dissipation:

Proposition 5 (Shape derivative). *The shape derivative of $\mathfrak{J}_{\Omega_\varepsilon}$ as given by (17) reads*

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon} = -\frac{G_\varepsilon}{\alpha} = -g_\varepsilon^* \cdot e \quad \text{where} \quad g_\varepsilon^* = \limsup_{\rho \rightarrow 0} \int_{\partial B_\rho^*} \Sigma(u_\varepsilon) n, \quad (39)$$

and with Σ given by (20).

The limit property in (39) will show crucial in the computation of the topological derivative.

4. TOPOLOGICAL SENSITIVITY ANALYSIS

The aim of the following sections is to analyse the energetical effect of infinitesimal crack nucleation at \hat{x} in a prescribed direction e . We will assume that there are no body forces.

In fact, we seek 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 (13) and (39) the topological derivative is introduced as

$$\text{TOPOLOGICAL DERIVATIVE} \quad D_T \psi = -\lim_{\varepsilon \rightarrow 0} \frac{\alpha}{f'(\varepsilon)} g_\varepsilon^* \cdot e. \quad (40)$$

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

$$\text{TOPOLOGICAL GRADIENT} \quad G_T \psi = -\lim_{\varepsilon \rightarrow 0} \frac{\alpha}{f'(\varepsilon)} g_\varepsilon^*. \quad (41)$$

The objective is now to compute rigorously the shape derivative in order to compute exact formulae for the topological derivative and gradient by using (40) and (41) and by means of an asymptotic analysis of the displacement around the crack tip. This analysis will be performed in the case of a bulk crack only.

4.1. Canonical problem. According to (6) & (9), let us define $v_\varepsilon := u_\varepsilon - u$, solution to

$$\begin{cases} -\operatorname{div} \sigma(v_\varepsilon) = 0 & \text{in } \Omega_\varepsilon \\ v_\varepsilon = 0 & \text{on } \Gamma_D \\ \sigma(v_\varepsilon) n = 0 & \text{on } \Gamma_N \\ \sigma(v_\varepsilon) e^\perp = -\sigma(u) e^\perp & \text{on } \gamma_\varepsilon \end{cases} \quad (42)$$

Moreover, let us introduce a microscopic variable $y := (x - x^*)/\varepsilon$ in order to re-scale the problem with a unit crack γ in \mathbb{R}^2 as $\varepsilon \rightarrow 0$. Indeed, it suffices to analyse the *canonical problem*

$$\begin{cases} -\operatorname{div}(\sigma(w)) = 0 & \text{in } \mathbb{R}^2 \\ \sigma(w) e^\perp = -\sigma(u)(x^*) e^\perp & \text{on } \gamma \end{cases} \quad (43)$$

which is well posed in the following Hilbert space (so-called Deny-Lions or Beppo-Levi space)

$$W := \{w \in H_{loc}^1(\mathbb{R}^2; \mathbb{R}^2) \text{ such that } \nabla^s w \in L^2(\mathbb{R}^2; \mathbb{R}^{2 \times 2})\}, \quad (44)$$

The solution of (43) is known as the Westergaard solution and reads (see, e.g., [65]), as a function of the complex variable $Z := y_1 + iy_2$:

$$2\mu w_1(Z) = \frac{\kappa - 1}{2} \Re\{\phi_I\} + \frac{\kappa + 1}{2} \Re\{\phi_{II}\} - y_2 \Im\{\phi'_I + \phi'_{II}\} \quad (45)$$

$$2\mu w_2(Z) = \frac{\kappa + 1}{2} \Im\{\phi_I\} + \frac{\kappa - 1}{2} \Im\{\phi_{II}\} - y_2 \Re\{\phi'_I + \phi'_{II}\} \quad (46)$$

with $\kappa = 3 - 4\nu$ in plane strains and $\kappa = (3 - \nu)/(1 + \nu)$ in plane stresses, and

$$\phi'_I(Z) + i\phi'_{II}(Z) = (K_I(u, e) - iK_{II}(u, e)) \left(\frac{Z}{\sqrt{Z^2 - a^2}} - 1 \right) \quad (47)$$

$$\phi_I(Z) + i\phi_{II}(Z) = (K_I(u, e) - iK_{II}(u, e)) \left(\sqrt{Z^2 - a^2} - Z \right) + C \quad (48)$$

given in terms of a constant C and the (normalized) *stress intensity factors*:

$$K_I(u, e) := \sigma(u)(x^*)e^\perp \cdot e^\perp \quad \text{and} \quad K_{II}(u, e) := \sigma(u)(x^*)e \cdot e^\perp. \quad (49)$$

4.2. Asymptotic analysis at the crack tip. Let us first mention that the displacement (45)-(46) shows by an asymptotic analysis of (47) and (48) around the crack tip x^* to be of the form

$$w := \Theta^* \bar{w} + \tilde{w} \quad (50)$$

where the cut-off function $\Theta^* \in \mathcal{C}_c^\infty(\mathbb{R}^2)$ verifies $\Theta^* \equiv 1$ in a neighborhood of x^* and

$$\bar{w}(y) := \sqrt{R}\psi(\Theta) \quad (51)$$

with $y_1 + iy_2 = Re^{i\Theta}$ and (R, Θ) the polar coordinates centered at x^* . Moreover, from [39] it is known that $\tilde{w} \in H_{loc}^2(\mathbb{R}^2) \cap W$.

Let us now observe that the re-scaled function

$$w_\varepsilon := \varepsilon w \left(\frac{x - x^*}{\varepsilon} \right) \quad (52)$$

solves

$$\begin{cases} -\operatorname{div}(\sigma(w_\varepsilon)) = 0 & \text{in } \Omega_\varepsilon \\ \sigma(w_\varepsilon)e^\perp = -\sigma(u)(x^*)e^\perp & \text{on } \gamma_\varepsilon \end{cases} \quad (53)$$

with non homogeneous but “small” boundary conditions on $\partial\Omega$.

The function $\bar{w}_\varepsilon := \varepsilon \bar{w}((x - x^*)/\varepsilon)$ will be written in polar coordinates as

$$\bar{w}_\varepsilon = \bar{w}_\varepsilon^r(r, \theta)e_r + \bar{w}_\varepsilon^\theta(r, \theta)e_\theta, \quad (54)$$

where $\{e_r, e_\theta\}$ denotes the polar base located at the crack tip x^* , with $-\pi \leq \theta < \pi$ and $r = \|x - x^*\|$. Moreover w_ε will be split into mode I and mode II singular components \bar{w}_ε^I and \bar{w}_ε^{II} , and a regular part $\tilde{w}_\varepsilon := \varepsilon \tilde{w}((x - x^*)/\varepsilon) \in H^2(\Omega)$:

$$w_\varepsilon = \theta^* (\bar{w}_\varepsilon^I + \bar{w}_\varepsilon^{II}) + \tilde{w}_\varepsilon, \quad (55)$$

where $\theta^* \in \mathcal{C}_c^\infty(\Omega)$ is such that $\theta^* \equiv 1$ in a neighborhood of x^* . Furthermore, the results will be given explicitly for plane stresses and plane strains. As relying on (45)-(46) and (52), the following expressions of the singular parts \bar{w}_ε^I and \bar{w}_ε^{II} are found in [52].

4.2.1. Plane stress problem. For plane stress problem, we have the following asymptotic expansion for the solution \bar{w}_ε , valid for r “small enough” (in a “neighborhood” of x^*):

- for the mode I

$$\bar{w}_\varepsilon^{Ir}(r, \theta) = \frac{K_I(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (3 - \nu - (1 + \nu) \cos \theta) \cos\left(\frac{\theta}{2}\right), \quad (56)$$

$$\bar{w}_\varepsilon^{I\theta}(r, \theta) = -\frac{K_I(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (3 - \nu - (1 + \nu) \cos \theta) \sin\left(\frac{\theta}{2}\right), \quad (57)$$

- for the mode II

$$\bar{w}_\varepsilon^{\text{II}r}(r, \theta) = \frac{K_{\text{II}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (3\nu - 1 + 3(1 + \nu) \cos \theta) \sin\left(\frac{\theta}{2}\right), \quad (58)$$

$$\bar{w}_\varepsilon^{\text{II}\theta}(r, \theta) = -\frac{K_{\text{II}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (5 + \nu - 3(1 + \nu) \cos \theta) \cos\left(\frac{\theta}{2}\right), \quad (59)$$

where $K_{\text{I}}, K_{\text{II}}$ are the SIF given in terms of the background solution u (let us precise that a small mistake in [52] has been here corrected).

4.2.2. *Plane strain problem.* For plane strain problem, we have the following asymptotic expansion for the solution \bar{w}_ε , valid for r “small enough”:

- for the mode I

$$\bar{w}_\varepsilon^{\text{I}r}(r, \theta) = \frac{K_{\text{I}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (1 + \nu) (3 - 4\nu - \cos \theta) \cos\left(\frac{\theta}{2}\right), \quad (60)$$

$$\bar{w}_\varepsilon^{\text{I}\theta}(r, \theta) = -\frac{K_{\text{I}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (1 + \nu) (3 - 4\nu - \cos \theta) \sin\left(\frac{\theta}{2}\right), \quad (61)$$

- for the mode II

$$\bar{w}_\varepsilon^{\text{II}r}(r, \theta) = \frac{K_{\text{II}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (1 + \nu) (4\nu - 1 + 3 \cos \theta) \sin\left(\frac{\theta}{2}\right), \quad (62)$$

$$\bar{w}_\varepsilon^{\text{II}\theta}(r, \theta) = \frac{K_{\text{II}}(u, e)}{E} \sqrt{\frac{r\varepsilon}{2}} (1 + \nu) (4\nu - 5 + 3 \cos \theta) \cos\left(\frac{\theta}{2}\right), \quad (63)$$

where $K_{\text{I}}, K_{\text{II}}$ are the SIF given in terms of the background solution u .

4.2.3. *Crack tip expansion of the displacement.* The function w_ε as given by (52) is the leading term of a so-called asymptotic expansion for v_ε as stated by the following Lemma.

Lemma 6. *For any cut-off function $\theta^* \in C_c^\infty(\Omega)$ such that $\theta^* \equiv 1$ in a neighborhood of x^* , there exists a constant $C > 0$ independent of ε such that*

$$v_\varepsilon := u_\varepsilon - u = \theta^* w_\varepsilon + \delta, \quad (64)$$

with w_ε solution of (53) and

$$\|\delta\|_{H^1(\Omega)} \leq C\varepsilon. \quad (65)$$

Remark 7. *Another way of writing (64) in a neighborhood of x^* is*

$$u_\varepsilon = u + \bar{w}_\varepsilon + O_{H^1}(\varepsilon), \quad (66)$$

with \bar{w}_ε given in a neighborhood of x^* in plane strains by (56)-(59) and in plane stresses by (60)-(63), with $u \in H^2(\Omega)$ the solution of the background problem. In fact it is easily verified that

$$\|\tilde{w}_\varepsilon\|_{H^1(\Omega)}^2 \leq C \int_\Omega |\nabla^s \tilde{w}_\varepsilon|^2 dx = C\varepsilon^2 \int_{\Omega/\varepsilon} |\nabla^s \tilde{w}|^2 dy \leq C\varepsilon^2.$$

Remark 8. *The role of the cut-off function is twofold: (i) to disregard the boundary behaviour of w_ε , and (ii) to localize the evaluation of the displacement in a neighborhood of x^* such that explicit expressions hold.*

Proof. According to (42) and (53), δ is the solution to

$$\begin{cases} -\operatorname{div}\sigma(\delta) = f_\varepsilon & \text{in } \Omega_\varepsilon \\ \delta = 0 & \text{on } \Gamma_D \\ \sigma(\delta)n = 0 & \text{on } \Gamma_N \\ \sigma(\delta)e^\perp = g_\varepsilon & \text{on } \gamma_\varepsilon \end{cases}. \quad (67)$$

where

$$f_\varepsilon := -\operatorname{div}[\mathbb{C}(\nabla\theta^* \otimes w_\varepsilon)^s + \sigma(w_\varepsilon)\theta^*] \quad (68)$$

$$g_\varepsilon := \sigma(u)(x^*)e^\perp - \sigma(u)e^\perp. \quad (69)$$

By multiplying (67) by δ and integrating by parts it results that

$$\int_{\Omega} \sigma(\delta) \cdot \nabla^s \delta = \int_{\Omega} f_{\varepsilon} \cdot \delta + \int_{\gamma_{\varepsilon}} g_{\varepsilon} \cdot \delta. \quad (70)$$

Let us remark that for some non negative constant C ,

$$\|g_{\varepsilon}\|_{\infty} \leq C\varepsilon \quad (71)$$

by the regularity of the background solution at x^* . Moreover by developing f_{ε} and noting that θ^* has a compact support in Ω , it results that

$$\int_{\Omega} f_{\varepsilon} \cdot \delta = \int_{\Omega} \mathbb{C}(\nabla\theta^* \otimes w_{\varepsilon})^s \cdot \nabla^s \delta - \int_{\Omega} (\sigma(w_{\varepsilon})\nabla\theta^* \cdot \delta - \sigma(w_{\varepsilon}) \cdot \theta^* \nabla^s \delta). \quad (72)$$

Let us also remark that

$$\|w_{\varepsilon}\|_{L^2(\Omega)}, \|\nabla w_{\varepsilon}\|_{L^2(\Omega)}, \|\sigma(w_{\varepsilon})\|_{L^2(\Omega)} \leq C\varepsilon \quad (73)$$

since for a non negative constant denoted by the generic symbol C , we have

$$\|w_{\varepsilon}\|_{L^2(\Omega)}^2 \leq C\|\nabla w_{\varepsilon}\|_{L^2(\Omega)}^2 \leq C\|\nabla^s w_{\varepsilon}\|_{L^2(\Omega)}^2 = C \int_{\Omega} |\nabla^s w_{\varepsilon}|^2 dx = C\varepsilon^2 \int_{\Omega/\varepsilon} |\nabla^s w|^2 dy \leq C\varepsilon^2$$

where the 3 inequalities follows from Poincaré and Korn inequalities, and by (44), respectively. Hence by (72) and (73) and observing that $\delta \in H^1(\Omega) \cap H^{1/2}(\gamma_{\varepsilon})$ verifies $\|\delta\|_{H^{1/2}(\gamma_{\varepsilon})} \leq C\|\delta\|_{H^1(\Omega)}$, it results that

$$C\|\nabla^s \delta\|_{L^2(\Omega)}^2 \leq (C'\varepsilon + C''\varepsilon^{3/2}) \|\nabla^s \delta\|_{L^2(\Omega)}$$

for some non negative constants C' and C'' , and hence that

$$\|\nabla^s \delta\|_{L^2(\Omega)} \leq C\varepsilon \quad (74)$$

for some non negative constant C , achieving the proof. \square

4.3. Estimation of the shape derivative. Let us recall that by Proposition 5 the shape derivative $\hat{\mathcal{J}}_{\Omega_{\varepsilon}}$ can be computed on any loop around x^* . Therefore, consider a family of balls $\{B_{\rho}(x^*); \rho\}$ such that $\theta^*(\{B_{\rho}; \rho\}) = 1$ and that (56)-(63) hold in $\cup_{\rho} B_{\rho}(x^*)$. Hence by (64), and by defining $\tilde{u} := u + \tilde{w}_{\varepsilon}$ we have

$$\hat{\mathcal{J}}_{\Omega_{\varepsilon}}(u_{\varepsilon}) = -e \cdot \limsup_{\{B_{\rho}(x^*); \rho\}} \int_{\partial B_{\rho}(x^*)} \Sigma(\bar{w}_{\varepsilon} + \tilde{u} + \delta)n. \quad (75)$$

On the other hand, according to (20), $\Sigma(v + w) = \Sigma_{\varepsilon}(v) + \Sigma_{\varepsilon}(w) + A(v, w)$ where

$$A(v, w) := \frac{1}{2}(\sigma(v) \cdot \nabla^s w + \sigma(w) \cdot \nabla^s v)I - \nabla v^T \sigma(w) - \nabla w^T \sigma(v) \quad (76)$$

Since f_{ε} vanishes near x^* it results from classical regularity that $\delta \in \mathcal{C}_{loc}^{\infty}(B_{\rho} \setminus \gamma_{\varepsilon})$ and $\nabla \delta \in \mathcal{C}(\partial B_{\rho})$. By (56)-(63) we have

$$\int_{\partial B_{\rho}} \Sigma(\bar{w}_{\varepsilon}) = O(\varepsilon) \quad (77)$$

where the left hand-side is independent of ρ . In addition, by the regularity of \tilde{u}, δ on ∂B_{ρ} ,

$$\int_{\partial B_{\rho}} \Sigma(\delta) = O(\rho), \int_{\partial B_{\rho}} \Sigma(u + \tilde{w}_{\varepsilon}) = O(\rho), \int_{\partial B_{\rho}} A(\tilde{u}, \delta) = O(\rho) \quad (78)$$

Moreover, by expressions (56)-(63),

$$\int_{\partial B_{\rho}} A(\tilde{u}, \bar{w}_{\varepsilon}) = O((\rho\varepsilon)^{1/2}), \int_{\partial B_{\rho}} A(\bar{w}_{\varepsilon}, \delta) = O((\rho\varepsilon)^{1/2}). \quad (79)$$

By (75)-(79), for every admissible ρ (i.e. such that $\theta^*(B_{\rho}) = 1$), we have

$$\hat{\mathcal{J}}_{\Omega_{\varepsilon}}(u_{\varepsilon}) + e \cdot \int_{\partial B_{\rho}} \Sigma(\bar{w}_{\varepsilon})n = O(\rho) + O((\rho\varepsilon)^{1/2}), \quad (80)$$

Since $\rho \ll \varepsilon < 1$, we can take a particular sequence $\rho = O(\varepsilon^2)$ satisfying $\theta^*(B_\rho) = 1$, to obtain

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -e \cdot \int_{\partial B_{\rho^*}} \Sigma(\bar{w}_\varepsilon)n + o(\varepsilon), \quad (81)$$

for any ρ^* satisfying $\theta^*(B_{\rho^*}) = 1$ (this choice is arbitrary since the first term on the right hand-side of the above equation is independent of ρ).

4.4. Topological derivative expression. From the formulas (56)-(63), we can solve the integral (81), which results in

$$\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -2\pi\varepsilon \frac{\varrho}{4E} (K_I^2 + K_{II}^2) + o(\varepsilon). \quad (82)$$

where $\varrho = 1$ in plane stresses, $\varrho = 1 - \nu^2$ in plane strains. It results that from expression (40) providing the topological derivative from the shape derivative, i.e. from equation (82), we can identify function $f'(\varepsilon) = 2\pi\varepsilon$ ($f(\varepsilon) = \pi\varepsilon^2$) and calculate the limit $\varepsilon \rightarrow 0$ in (40), that is

$$D_T\psi(u, e) = \lim_{\varepsilon \rightarrow 0} \frac{\alpha}{f'(\varepsilon)} \dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon) = -\frac{\alpha\varrho}{4E} (K_I^2 + K_{II}^2) \quad (83)$$

while by (41), the topological gradient reads

$$G_T\psi(u, e) = D_T\psi(u, e)e. \quad (84)$$

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

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2 \frac{\alpha\varrho}{4E} (K_I^2 + K_{II}^2) + o(\varepsilon^2). \quad (85)$$

5. MINIMAL TOPOLOGICAL DERIVATIVE AS A CRACK NUCLEATION CRITERION

The above analysis provides a new feature: for cracks of vanishing length, a precise notion of topological derivative – given by (83) – has been introduced. As far as the total potential energy $\dot{\mathfrak{J}}_{\Omega_\varepsilon}(u_\varepsilon)$ is concerned, the explicit expression (83) shows that its topological derivative is always negative, which means that the presence of a crack of any length anywhere in Ω provides a lower total potential energy as compared to that of the uncracked body. This property is completely natural since nucleation means extending the class of candidates for the minimization of (10) with those candidates allowed to jump across the crack lips. To that extend, the topological derivation has not brought significant insight to the issue of crack nucleation.

However it results that from the notion of topological derivative, the principle of maximal dissipation or, equivalently, of minimal topological derivative, provides a crack nucleation criterion. In fact, (83) provides an explicit criterion for the determination of the weakest zones in Ω with respect to crack initiation, in the sense that optimal nucleation points x^* and orientation $e(\varphi^*)$ may be sought to satisfy:

$$\text{NUCLEATION CRITERION } D_T\psi(x^*, e(\varphi^*)) = \min_{x \in \Omega, \varphi \in [0; 2\pi[} D_T\psi(x, e(\varphi)), \quad (86)$$

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

The above criterion (86) is only apparently based on a double minimization. It 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. In fact, the nucleation criterion only amounts to the minimization of the scalar field $D_T\psi(x, e(\varphi^*))$ over $x \in \Omega$ because there exist a law providing optimal fracture direction (i.e., the angle φ^*).

It can be observed that the nucleation optimality criterion (86) is, by (13) and (82), 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 [27, 46, 50, 52], it is here given a precise mathematical meaning, and proven.

Let us remark that the introduction of a precise notion of derivation for crack nucleation is justified also by the fact that from the sole Griffith's critical relation:

$$G_\varepsilon = 2\pi\varepsilon \frac{K_I^2 + K_{II}^2}{E} = G_{crit}, \quad (87)$$

where G_{crit} is a material dependent crack growth threshold, one would deduce 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 $\varepsilon \rightarrow 0$.

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 [52], it is not specifically dedicated for crack nucleation predictions. Let us 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 [2].

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

5.1. Case 1: bulk crack initiation. Let us fix \hat{x} in Ω , and take $\alpha = 2$ in order to account for the crack symmetry property. According to the classical expressions of the SIF as given by (49), it results that the topological derivative writes

$$D_T\psi = -\frac{\varrho}{2E} \left[(\sigma(u)e^\perp \cdot e^\perp)^2 + (\sigma(u)e \cdot e^\perp)^2 \right], \quad (88)$$

where $\varrho = 1$ in plane stresses, $\varrho = 1 - \nu^2$ in plane strains.

The crack will nucleate according to the above criterion (86) in a direction which minimizes the topological derivative. Hence, by writing

$$e = (\cos \varphi, \sin \varphi) \quad \text{and} \quad e^\perp = (-\sin \varphi, \cos \varphi), \quad (89)$$

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 φ^* such that

$$\varphi^* := \arg \left\{ \max_{0 \leq \varphi < 2\pi} \left[\sigma_{11}^2 + 2\sigma_{12}^2 + \sigma_{22}^2 + (\sigma_{22}^2 - \sigma_{11}^2) \cos(2\varphi) - 2\sigma_{12}(\sigma_{11} + \sigma_{22}) \sin(2\varphi) \right] \right\}, \quad (90)$$

which results in

$$\varphi^* = \pm \frac{1}{2} \arccos \left(\pm \sqrt{\frac{(\sigma_{11} - \sigma_{22})^2}{(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}^2}} \right) \quad (91)$$

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

Therefore, according to the above topological minimization framework, the so-called ‘‘local symmetry principle’’ (see the pioneering works [16, 29, 37] and the recent discussion [25], otherwise called ‘‘ $K_{II} = 0$ nucleation criterion’’, instead of being simply postulated, can now be proved.

Proposition 9 ($K_{II} = 0$ nucleation criterion). *In homogeneous LEFM, the $K_{II} = 0$ crack nucleation criterion satisfies the property of minimal topological derivative, i.e., of maximal decrease of the total potential energy (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 (91) results in $\varphi^* = 0$ or $\pi/2$. Clearly, since $e_2^\perp = e_1$, the lowest value of the topological derivative is attained for $\varphi^* = \pi/2$. \square

The local symmetry principle is sometimes called $K_{II} = 0$ criterion because 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 only, whereas for cracks of finite length, other physical mechanisms should be taken into account [21,33]. Let us also mention that, unless the presence of impurities, brittle crack initiation in the sense of Griffith always implies cracks of finite length, as discussed in [21] or [26], and hence at nucleation points, no infinitesimal crack will ever appear. This latter property will also appear clear and be proven within our setting in section 6.

As a matter of fact, Proposition 9 also contributes to the debate between the validity of Irwin's maximal dissipation criterion versus the local symmetry principle. In fact, Proposition 9 states that relying on Irwin's principle, a precise notion of nucleation is introduced via the topological derivative, whose minimal value coincides with the $K_{II} = 0$ criterion and with the principle of maximal traction.

5.2. Case 2: boundary crack initiation. In this case, $\hat{x} \in \partial\Omega$, there is one crack extremity at the boundary while the other is located inside the body, i.e. $\alpha = 1$. Moreover, since the domain boundary was assumed smooth, the canonical problem results in a semi-infinite crack with endpoint x^* in a semi-infinite plane. Let us consider (47) and (48) as developed in a neighborhood of x^* as functions of the SIF [65]:

$$\phi'_I(Z) + i\phi'_{II}(Z) = (K_I^* - iK_{II}^*) \frac{\exp(-i\Theta/2)}{\sqrt{2\pi}\sqrt{R}} \quad (92)$$

$$\phi_I(Z) + i\phi_{II}(Z) = (K_I^* - iK_{II}^*) \sqrt{\frac{2}{\pi}} \sqrt{R} \exp(i\Theta/2) + C. \quad (93)$$

In the rescaled domain where the boundary crack has length ε , the displacement are given by (56)-(59) provided K_I and K_{II} are replaced by K_I^* and K_{II}^* , respectively, with

$$\begin{pmatrix} K_I^* \\ K_{II}^* \end{pmatrix} = \begin{pmatrix} F_I^S & F_I^T \\ F_{II}^S & F_{II}^T \end{pmatrix} (\beta) \begin{pmatrix} \sigma(u)(x^*)e^\perp \cdot e^\perp \\ \sigma(u)(x^*)e \cdot e^\perp \end{pmatrix}, \quad (94)$$

where coefficients F_I^S, F_I^T and F_{II}^S, F_{II}^T depend on the angle β between the crack and the normal n to the boundary $\partial\Omega$ (approximate analytical expressions of these coefficients are given in [17]). Let us remark that for the simple case $\beta = \pi/2$ the SIF have been given in [64] as

$$K_I^* - iK_{II}^* = 1.1215 \left(\sigma(u)(x^*)e^\perp \cdot e^\perp - i\sigma(u)(x^*)e \cdot e^\perp \right).$$

According to the above general expression of the SIF, the topological derivative at $\hat{x} \in \partial\Omega$ reads

$$D_T\psi(\hat{x}) = -\frac{\varrho}{4E} \left[(F_I^S\sigma e^\perp \cdot e^\perp + F_I^T\sigma e \cdot e^\perp)^2 + (F_{II}^S\sigma e^\perp \cdot e^\perp + F_{II}^T\sigma e \cdot e^\perp)^2 \right] (u)(\hat{x}),$$

where $\varrho = 1$ in plane stresses, $\varrho = 1 - \nu^2$ in plane strains.

Provided the approximate analytical expressions as found in [17], the calculation of the optimal angles φ^* can be done by following exactly the same steps as presented in the previous case.

5.3. Case 3: kinking. The case of kinking can in principle be addressed by our method. Let us consider an elastic body with a pre-existing crack γ with tip \hat{x}^* and an extension γ_ε of that crack at \hat{x}^* whose tip is denoted x^{**} and which forms an angle ζ with the direction tangent to γ at \hat{x}^* . It was shown in [4] that for small kinking angles the displacement are given by (56)-(59) provided K_I and K_{II} are replaced by K_I^{**} and K_{II}^{**} , respectively, with

$$\begin{pmatrix} K_I^{**} \\ K_{II}^{**} \end{pmatrix} = \mathcal{G}(\zeta) \begin{pmatrix} K_I^* \\ K_{II}^* \end{pmatrix},$$

where K_I^* and K_{II}^* are the SIF of γ at \hat{x}^* . Several exact expressions of the matrix \mathcal{G} are given in [5] for particular kink configurations.

However, it should be remarked that these formulae are based on the postulate that kinking occurs according to the principle of local symmetry. Here we have proved that bulk crack nucleates according to that principle, but have not extended that property to general crack growth. As a matter of fact, it should be verified that minimizing the topological derivative in the case of kinking is equivalent to the local symmetry principle. Since arguments are found in [25] to believe in a negative answer to that latter assertion, our method of minimal topological derivative as applied to kinking remains questionable.

6. 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 other types of energy-based shape functionals, let us consider the Griffith's-type surface energy of the form

$$\Xi(\Omega_\varepsilon) = \psi(\Omega_\varepsilon) + C(\gamma_\varepsilon) , \quad (95)$$

with

$$C(\gamma_\varepsilon) = \int_{\gamma_\varepsilon} \kappa(\varepsilon) , \quad (96)$$

whose simplest expression is taken as

$$C(\gamma_\varepsilon) = \tilde{\kappa}\varepsilon , \quad (97)$$

where $\tilde{\kappa} > 0$ is the specific (material dependent) surface energy. The solutions to the associated elastic problem, obtained by a global minimization approach [21], here satisfy (9).

From (97) it follows that the derivative w.r.t. ε of $C(\gamma_\varepsilon)$ is given by

$$\dot{C}(\gamma_\varepsilon) = \tilde{\kappa} > 0 . \quad (98)$$

whereby from (85) and (98) it results that $\Xi(\Omega_\varepsilon)$ admits the following total derivative w.r.t. ε :

$$\dot{\Xi}(\Omega_\varepsilon) = \tilde{\kappa} + O(\varepsilon) , \quad (99)$$

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

$$D_T \Xi = \lim_{\varepsilon \rightarrow 0} \left(\frac{1}{f'_\Xi(\varepsilon)} \dot{\Xi}(\Omega_\varepsilon) \right) = \tilde{\kappa} > 0 . \quad (100)$$

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 10. *In homogeneous LEFM, according to the topological derivative criterion (86) as applied to (95) and (97), there will be no infinitesimal crack nucleation.*

The above property appears as another proof of a result found in [21] 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 ε^* can be explicitly bounded from below. In fact, the topological asymptotic expansion of the shape functional (95) reads

$$\Xi(\Omega_\varepsilon) = \Xi(\Omega) + \varepsilon\tilde{\kappa} + \pi\varepsilon^2 D_T \psi + o(\varepsilon^2) . \quad (101)$$

where $D_T \psi$ can be obtained from (85). Hence, as a result of the balance between potential and surface energy contributions, the following thresholds are found:

$$\varepsilon^* > \frac{2\tilde{\kappa}E}{\pi\varrho K_I^2} , \quad (102)$$

where $\varrho = 1$ in plane stresses, $\varrho = 1 - \nu^2$ in plane strains. In fact, it suffices to observe that according to Proposition 9 $\varphi^* = \pi/2$ and $K_{II} = 0$.

7. CONCLUSIONS

In this paper, we mainly provide a simple tool justified by a rigorous mathematical approach, aimed at analysing variational brittle crack nucleation 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 recognized as the total potential energy of an elastic cracked body. The case of bulk and surface energy contributions of Griffith-type has also been addressed.

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 referred to as postulates, or principles.

As main results we have mathematically formulated a crack nucleation criterion based on the notion of topological derivative and a criterion for determining the direction of crack growth based on the topological gradient, and showed how these criteria coincide with the principle of maximal dissipation. In particular we have proved that in order to maximize dissipation at a bulk point of the solid the crack will nucleate in pure mode II. Moreover, for Griffith's model where a competition between a volume and a surface energy is considered, crack nucleation is proven to occur brutally.

In addition, 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) not restricted to a given physical model of brittle fracture. As a matter of fact, provided the solution to a modified primal perturbed problem (9) is given as an asymptotic expression in terms of the small crack length ε , then the proposed framework can be applied, resulting in appropriate nucleation criteria. Moreover, it is clear that other shape functional than the potential or Griffith energy can freely be chosen within our setting, provided they admit a topological derivative.

As a consequence, our methodology provides a family of nucleation criteria – according to the chosen model of brittle fracture, which can be further tested and compared by laboratory or numerical experiments.

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