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Configurational Forces and a Constitutive Theory for Crack Propagation that Allows for Kinking and Curving

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CONFIGURATIONAL FORCES AND A CONSTITUTIVE THEORY FOR CRACK PROPAGATION THAT ALLOWS FOR KINKING AND CURVING

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ABSTRACT This paper develops a framework for dynamical fracture, concentrating on the derivation of balance equations and constitutive equations that describe the motion of the crack tip in two space-dimensions. The theory is based on the notion of configurational forces in conjunction with a mechanical version of the second law. Kinking and curving of the crack are allowed under the assumption that the crack will propagate in a direction that maximizes the rate at which it dissipates energy.

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1. INTRODUCTION

This paper is a continuation of a program, begun in (1996),¹ whose goal is a general framework for brittle fracture based on the notion of configurational forces in conjunction with a mechanical version of the second law of thermodynamics. Here we extend the framework developed in (1996) in two directions:

- (i) In (1996) we neglected the energy of the crack surfaces. Here we include what we believe to be all relevant energies and forces.
- (ii) We discuss at length propagation of a running crack, crack initiation with and without kinking, and crack curving. These central issues in fracture mechanics (vid. FREUND (1990)) are here regarded as constitutive, and are accordingly discussed as such.

We work within the theory of finite deformations, because the basic ideas are most easily explained when there is a clear distinction between reference and deformed configurations. As noted in (1996), our analysis is applicable with only minor modification to small strains.

Our study is divided into three parts. Part I covers the geometry and the kinematics of a cracked body; Part II, the standard and configurational force systems in a cracked body, and their balance and imbalance laws; Part III is devoted to the constitutive aspects of crack propagation. The main contents of the three parts may be summarized as follows.

a. Part I

We view a two-dimensional cracked body B as a referential neighborhood of a two-face curve with one end fixed at the boundary ∂B of B while the other end, the crack tip, is contained in the interior of B and has a velocity $\mathbf{v} = \mathbf{V}\mathbf{e}$, with $\mathbf{V} \ge 0$ the tip speed and \mathbf{e} the direction of propagation.

A tool we recurrently use to describe the kinematics and the dynamics of cracked bodies is the notion of a *migrating control volume* R(t); an especially important example of a migrating control volume is a *tip disc* $D_{\delta}(t)$, which is a disc of radius δ centered at the tip and moving with it. Another tool we utilize, in this paper as in (1996), is the notion of a *tip integral*

$$\oint_{tip} \{ \dots \} n = \lim_{\delta \to 0} \int \{ \dots \} n, \qquad D_{\delta} = D_{\delta}(t),$$

where n is the outward unit normal to ∂D_{δ} , and $\{...\}$ denotes an arbitrary integrand. With these ingredients and tools, a number of *transport theorems* are $\frac{1}{(1996)}$ (without names) signifies GURTIN and PODIO-GUIDUGLI (1996).

derived.

b. Part II

A notion central to our account of the phenomenology of cracking, is that of a system of configurational forces.

As customary in continuum mechanics, we describe the response of a body to deformation by a system of standard (newtonian) forces. We relate configurational forces to the coherency of a body's material structure and hence stipulate that they perform work in the addition and removal of material and in the evolution of structural defects. Following GURTIN and STRUTHERS (1990) and GURTIN (1995,1997), we view configurational forces as primitive objects consistent with their own balance. That configurational forces may be needed to describe the internal structure of the material follows from the beautiful work of ESHELBY (1951,1956,1970) on lattice defects and fracture.² But Eshelby's studies are statical, based on variational arguments, with configurational forces defined as derivatives of the energy; for that reason Eshelby does not need a balance law for configurational forces, a law that to us is essential to the description of time-dependent, dissipative phenomena.

The ingredients of the configurational force system we envisage consist of a bulk stress C, an internal force g_{int} concentrated at the crack tip, a surface tension σ that acts within the free surfaces of the crack, and other less important forces discussed in the text. We associate g_{int} with the breaking of bonds during crack growth or, more generally, to phenomena occuring at the tip at length scales small compared to the gross length scale of the body.³ The surface tension σ is purely configurational; in fact, we here choose not to include surface tension in the standard force-system.⁴

Essential to the theory are the (dynamical) tip traction j and the energy release rate⁵ J, defined by

²Cf. MAUGIN (1993,1995) for a discussion of configurational forces within an Eshelbian framework, and for related references.

³Cf. the discussion of FREUND (1990, pp. 10-11). An example of such phenomena is "small-scale yielding" associated with a crack-tip plastic zone (RICE, 1968).

⁴To allow for surface tension in the standard force system would necessitate straindependent surface energies (GURTIN and STRUTHERS, 1990; GURTIN 1995). To quote HERRING (1951a) on crystalline materials: "the principal cause of surface tension is the fact that surface atoms are bound by fewer neighbors than internal atoms; surface tension is therefore mainly a measure of the change in the number of atoms in the surface layer." We interpret this as inferring that surface tension in crystalline materials is primarily configurational.

⁵A concept introduced by ATKINSON and ESHELBY (1968) and justified by FREUND (1972); cf. FREUND (1990, pp. 221-235). Within the framework of quasi-static elasticity

$$\mathbf{j} = \oint_{\mathrm{tip}} \{ (\Psi + \mathbf{k}_{\mathrm{rel}}) \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}, \qquad \mathbf{J} = \mathbf{e} \cdot \mathbf{j} = \mathbf{e} \cdot \oint_{\mathrm{tip}} \{ (\Psi + \mathbf{k}_{\mathrm{rel}}) \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}.$$

Here Ψ is the (bulk) free energy density, **S** is the standard stress, \mathbf{F}^{T} is the transpose of the deformation gradient **F**, **1** is the unit tensor, and \mathbf{k}_{rel} is the kinetic energy measured relative to the deformed crack tip. The vector **j** represents the configurational traction $\oint_{tip} \mathbf{Cn}$ on the material in an infinitesimal neighborhood of the tip, augmented by an "inertial traction" $\oint_{tip} \mathbf{k}_{rel}\mathbf{n}$. The scalar J is the component of **j** in the direction of propagation.

The manifestation of the configurational force balance most relevant to the motion of the tip is the localization, to an infinitesimal neighborhood of the tip, of its component in the direction of propagation:

$$J - \psi_{tip} + \mathbf{e} \cdot \mathbf{g}_{int} = 0, \tag{1.1}$$

where ψ_{tip} represents the energy (= surface tension) of the crack surfaces at the tip. This relation may be regarded as a balance between $-\mathbf{e}\cdot\mathbf{g}_{int}$, the internal force that opposes motion of the tip, and $f = J - \psi_{tip}$, the driving force for crack propagation.

We supplement the configurational force balance with a mechanical version of the second law; the localization of this law to the tip yields the simple but important inequality, $\Gamma_{tip} = -(\mathbf{e} \cdot \mathbf{g}_{int}) \nabla = f \nabla \ge 0$, where Γ_{tip} is the energy dissipated at the tip, per unit time. We view this inequality as indication of a need for (suitably restricted) constitutive assumptions involving V and $\mathbf{e} \cdot \mathbf{g}_{int}$.

We believe it important to differentiate between the roles played by the quantities appearing in (1.1). In the literature one typically finds constitutive prescriptions for J. Our view is that $\mathbf{e} \cdot \mathbf{g}_{int}$ and ψ_{tip} are constitutive, with J a defined quantity related to $\mathbf{e} \cdot \mathbf{g}_{int}$ and ψ_{tip} through the balance (1.1). To us the prescription of a constitutive equation for J masks both the presence of the configurational force balance and the existence the internal configurational force \mathbf{g}_{int} , a physically significant quantity.

c. Part III

The last part of our study concerns the *constitutive* aspects of crack propagation. Here we believe our chief contributions to be:

(i) A fairly complete constitutive theory for the tip with results independent of bulk constitution.

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the basic ideas are inherent in the work of ESHELBY (1956) and RICE (1968); there the energy release rate coincides with the path-independent J-integral.

- (ii) A treatment of anisotropy in the free energy of the crack surfaces and in the constitutive description of the kinetics of the tip.
- (iii) A criterion for crack-initiation that allows for kinking.
- (iv) A criterion for determining the direction of a running crack; in contrast to previous criteria based on minimizing the energy release rate, ours selects directions that maximize dissipation.

We depart from standard fracture theories by allowing the free energy of the crack surface to depend on its orientation as described by the angle θ of its tangent $\mathbf{e} = \mathbf{e}(\theta) = (\cos \theta, \sin \theta)$. More precisely, as we are primarily interested in the behavior of the tip, we consider a constitutive equation of the form

 $\psi_{tip} = \hat{\psi}(\Theta)$

for the tip surface energy ψ_{tip} . Surface energies in crystalline materials typically exhibit a strong dependence on orientation, and the stability of crystals is known to depend crucially on the convexity of such energies, with nonconvexity the rule rather than the exception (HERRING, 1951b; GJOSTEIN, 1963; CAHN and HOFFMAN, 1974; GURTIN, 1993). Here, because of periodicity, the description of convexity is not straightforward; using ideas originating in the materials science literature, we base our definition of convexity on the notion of a *Frank diagram* (FRANK, 1963), which, for an arbitrary function $\varphi(\theta)$, is the *curve* defined in polar coordinates (r,θ) by $r = \varphi(\theta)^{-1}$. We refer to $\varphi(\theta)$ as angle-convex if its Frank diagram, Frank(φ), is strictly convex.

To describe the kinetics of the crack tip we consider a constitutive equation giving the crack speed V when the angle θ and the driving force $f = J - \psi_{tip}$, are known.⁶ Here we assume that there is an orientation-dependent limit-force $F(\theta) > 0$, below which the tip is stationary, and therefore write the constitutive equation for V in the form:⁷

V	=	0	for	f	≤	F(0),
v	=	$\hat{V}(\Theta, f) > 0$	for	f	>	F(ə).

Central to our theory is the Griffith-Irwin function

⁶Basic here is the assumption $\oint_{tip} p\mathbf{y} \cdot \otimes \mathbf{n} = \mathbf{0}$, which is satisfied when $\mathbf{y}^* = O(r^{-p})$, p < 1. In linear elasticity, $\mathbf{p} = \frac{1}{2} (cf., e.g., FREUND, 1990, \$1.4.3, \$4)$.

⁷When orientational aspects are not considered, the experimental results of ROSAKIS *et al.* (1984) and ZENDER and ROSAKIS (1990) as displayed in Figure 11 of the latter paper, at least indicate behavior of this form, as does the micromechanical model of LAM and FREUND (1985) (FREUND, 1990, \$8.3).

$$\Phi(\Theta) := \hat{\psi}(\Theta) + F(\Theta) > 0. \tag{1.2}$$

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As the propagation condition $f > F(\theta)$ is equivalent to $J(\theta, \mathbf{j}) > \Phi(\theta)$, where $J(\theta, \mathbf{j}) = \mathbf{e}(\theta) \cdot \mathbf{j}$, the classical Griffith criterion $J(\theta, \mathbf{j}) > \hat{\psi}(\theta)$ is conservative within our framework.

The issue of crack initiation, i.e., the onset of propagation for a stationary crack, possibly with the formation of an initial kink, is discussed by making extensive use of the notion of angle-convexity of the Griffith-Irwin function $\Phi(\theta)$ and of the Frank diagrams of both $\Phi(\theta)$ and the energy release rate $J(\theta)=J(\theta,j)$ at a fixed tip traction j. In fact, these concepts allow for a complete geometric picture of the qualitative aspects of the fracture process. A stationary crack will remain stationary as long as the straight line Frank(J) remains strictly outside the closed curve Frank(Φ). Initiation of a running crack begins at a time for which Frank(J) passes across Frank(Φ), with a portion of Frank(J) entering the open region interior to Frank(Φ); and the crack will continue to run as long as a portion of Frank(J) remains interior to Frank(Φ). At the time of initiation Frank(J) touches Frank(Φ), but has no intersection with its interior the possible kink angles are those angles θ^+ that mark the intersection of Frank(Φ) with Frank(J). In this latter case there may be many such angles θ^+ , possibly infinitely many; we prove that each possible kink angle θ^+ is related to j through⁸

$$\mathbf{j} = \Phi(\Theta^+) \mathbf{e}(\Theta^+) + \Phi'(\Theta^+) \mathbf{m}(\Theta^+), \tag{1.3}$$

with $m(\theta^*)$ the normal to the crack at the tip. We show further that there is at most one possible kink angle when the Griffith-Irwin function $\Phi(\theta)$ is angle-convex. Our results show that in general one should not expect the crack to initiate aligned with the tip traction, although this is always the case for constitutively isotropic tips, whose Griffith-Irwin function is, in fact, a material constant.

We propose a criterion of maximum dissipation, which postulates that, at each fixed time t, a crack advance at an angle $\theta(t)$ that solves the extremum problem

$$\Gamma_{\rm tip}(\mathbf{j}, \theta) = \max_{\alpha \in G(\mathbf{j})} \Gamma_{\rm tip}(\mathbf{j}, \alpha), \qquad G(\mathbf{j}) = \{ \text{angles } \theta \text{ such that } J(\mathbf{j}, \theta) > \Phi(\theta) \}.$$

A thermodynamical statement of this criterion is that, under isothermal condi-⁸Interestingly, surface stress and surface free energy are related through an identical relation (cf. Remark 7.1). tions, a crack propagate in a direction that maximizes the entropy production at the tip. A main implication of the maximum dissipation criterion is that anisotropy generally induces an angle discrepancy between the tip traction and the direction of propagation. For a class of crack tips with $\hat{V}(\theta, f) = M[f-F(\theta)]$ for $f > F(\theta)$, which we refer to as tips with constant mobility M, the propagation angle is uniquely determined if Φ angle-convex; the same is true for a constitutively isotropic tip and in this case, as expected, the crack propagates in the direction of the tip traction.

To put the maximum dissipation criterion into perspective, we observe that arguments were given by COTTERELL (1965) in support of the requirement that the crack advance at an angle θ that maximizes the energy release rate $J(\mathbf{j},\theta)$.⁹ A possible extension of Cotterell's criterion to anisotropic tips asserts that the crack advance at an angle θ that maximizes the total energy release rate $J(\mathbf{j},\theta) - \hat{\psi}(\theta)$; for isotropic tips and for tips with both F and M constant such an extension yields predictions coincident with those of the maximum dissipation criterion, but in general the predictions of the two criteria are not the same.

Our final section contains a sketch of a promising application of our theory to the fracture of crystalline materials. The typical faceted shapes of those materials can be shown to be a consequence of restricting the function delivering the energy density of a free surface to a finite set of orientations. Likewise, we restrict the functions that specify a material's cracking response to Θ , here a finite set of angles, and we assume that the only impediment to fracture is the formation of new free surfaces, thus identifying for simplicity $\hat{\psi}(\theta)$, the tip surface energy, with the energy density on a crystal facet, and choosing $F(\theta) \equiv 0$. In addition, to further simplify our discussion, we assume that the mobility is constant. Cracks in such materials propagate without curving, changing their direction only by kinking; granted this, the qualitative picture of the fracture process is similar to that discussed above.

⁹Cf. HUSSAIN, PU, and UNDERWOOD (1974), PALANISWAMY and KNAUSS (1978), COTTERELL and RICE (1980), LE (1989ab), STUMPF and LE (1990,1992).

PART I. GEOMETRY AND KINEMATICS OF CRACKED BODIES

2. CRACKED BODIES

We begin with a discussion of smooth cracks. In future sections we will apply our results to crack kinking, an application that involves no inconsistency, as the evolution of the tip is governed by *local* physical laws that apply away from (although arbitrarily close to) points at which the crack kinks.

a. Smooth cracks. Migrating control volumes

Let B denote a closed region of \mathbb{R}^2 with boundary ∂B and, for each t in some open time interval, let C(t) be a smooth, connected, oriented curve in B with one end, \mathbf{Z}_0 , fixed at the boundary ∂B , with the remainder of $\mathbf{C}(t)$ — including the other end point Z(t) — contained in the interior of B, and with $C(\tau) \subset C(t)$ for all $\tau \leq t$. We view B as a referential neighborhood of a growing crack C(t) with Z(t) the crack tip (Figure 1). The phrase "in bulk" will be used to signify "away from the crack".

We measure arc length s from Z_0 , and write s(X) for the arc length to a point $X \in C(t)$. Let e(X) denote the unit tangent to C(t) in the direction of increasing s. Then, since e(Z(t)) represents the direction of (possible) propagation, the tip velocity

$$\mathbf{v}(t) = d\mathbf{Z}(t)/dt \tag{2.1}$$

may be written in the form

$$\mathbf{v}(t) = V(t) \mathbf{e}(\mathbf{Z}(t)), \quad V(t) \ge 0,$$
 (2.2)

with V the tip speed.

We let $\mathbf{m}(\mathbf{X})$ denote a continuous unit normal field for $\mathbf{C}(t)$.

By a (migrating) control volume¹⁰ we mean a closed subregion R(t) of B for which $\partial R(t)$ evolves smoothly with t, for which C(t) does not intersect $\partial R(t)$ at more than two points, and for which $Z(t) \notin \partial R(t)$. Then R(t) must be either:

(i) a bulk control-volume, which does not intersect the crack; or

(ii) a crack control-volume, which contains a portion of the crack, but not the

¹⁰In continuum mechanics one often uses the term part for a fixed subregion R of B; and by the phrase "evolution of R with time" one refers to the motion of the deformed part $\mathbf{y}(\mathbf{R},t)$. Parts should not be confused with control volumes $\mathbf{R}(t)$, which are not fixed subregions of the reference region B, but instead migrate through B.



Figure 1 Referential neighborhood of a growing crack.

tip; or

(iii) a tip control-volume, which contains the tip in its interior.

For R(t) a control volume, n(X,t) designates the outward unit normal to $\partial R(t)$, while $U_{\partial R}(X,t)$ is the (scalar) normal velocity of the boundary curve in the direction n(X,t) (cf. (3.2), (3.3)).

For R(t) a tip control-volume, C(t) intersects $\partial R(t)$ at a single point $X^{-}(t)$, and u-(t) defined by

$$(X^{-})^{*}(t) = u^{-}(t)e^{-}(t), e^{-}(t) = e(X^{-}(t))$$
 (2.3)

represents the velocity of $X^{-}(t)$. Similarly, when R is a crack control-volume, C(t) intersects $\partial R(t)$ at two points $X^{\pm}(t)$, and $u^{\pm}(t)$ defined by

$$(X^{\pm})^{\bullet}(t) = u^{\pm}(t)e^{\pm}(t), \qquad e^{\pm}(t) = e(X^{\pm}(t))$$
 (2.4)

is the velocity of $X^{\pm}(t)$, where, for definiteness,

$$s(X^{+}(t)) > s(X^{-}(t)).$$
 (2.5)

An important example of a tip control-volume is a tip disc $D_{\delta}(t)$ (Figure 2), which is a disc of radius δ centered at the tip Z(t); here, letting $n^{-}(t) = n(X^{-}(t),t)$,

$$U_{\partial D_{\delta}} = \mathbf{v} \cdot \mathbf{n}, \qquad u^{-} = U_{\partial D_{\delta}} / e^{- \cdot \mathbf{n}^{-}}, \qquad (2.6)$$

and, as $\delta \rightarrow 0$,

$$e^{-}(t) \rightarrow e(Z(t)), \qquad u^{-}(t) \rightarrow V(t).$$
 (2.7)

(Since $e^{-} \cdot n^{-} \rightarrow -1$, we choose δ small enough that $e^{-} \cdot n^{-} \neq 0$.)

An example of a crack control-volume is constructed as follows. Let $\mathcal{P}(t)$ denote an arbitrary connected subcurve of the crack, with $\mathbf{Z}(t) \notin \mathcal{P}(t)$. Then the *pillbox* $P_{s}(t)$ corresponding to $\mathcal{P}(t)$ is the region

$$P_{\delta}(t) = \{ \mathbf{X} \in \mathbb{B} : \mathbf{X} = \mathbf{X}^{*} + \alpha \mathbf{m}(\mathbf{X}), -\delta \le \alpha \le \delta, \mathbf{X}^{*} \in \mathcal{P}(t) \}$$
(2.8)

(Figure 2). Writing $X^{\pm}(t)$, $s(X^{-}(t)) > s(X^{+}(t))$, for the endpoints of $\mathcal{P}(t)$, and suppressing the argument t, ∂P_{δ} consists of:

(i) two curves, each parallel to—and a distance δ from— $\mathcal{P}(t)$; on these curves





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the normal velocity of ∂P_{δ} vanishes;

(ii) two end faces of length δ perpendicular to $\mathcal{P}(t)$, one at X^- , the other at X^+ .

b. Derivatives following the crack tip. Tip integrals. Transport theorems We refer to a field $\varphi(\mathbf{X},t)$ as smooth away from the tip if $\varphi(\mathbf{X},t)$ is defined away from the crack and if, away from the tip, $\varphi(\mathbf{X},t)$ and its derivatives have limits up to the crack from either side; we then write, for $\mathbf{X} \in \mathbb{C}(t)$,

$$[\varphi](\mathbf{X},t) = \lim_{\epsilon \to 0} \varphi(\mathbf{X} + \epsilon \mathbf{m}(\mathbf{X}),t) - \lim_{\epsilon \to 0} \varphi(\mathbf{X} - \epsilon \mathbf{m}(\mathbf{X}),t).$$
(2.9)

Given such a field $\varphi(X,t)$, consider the corresponding field $\hat{\varphi}(Y,t)$ in which Y represents the position of the material point X relative to the tip Z(t):

$$\hat{\varphi}(\mathbf{Y},t) = \varphi(\mathbf{X},t), \qquad \mathbf{Y} = \mathbf{X} - \mathbf{Z}(t).$$
 (2.10)

The partial derivative

$$\varphi^{\circ}(\mathbf{X},t) = \partial \hat{\varphi}(\mathbf{Y},t) / \partial t$$

with respect to t holding Y fixed represents the time derivative of $\varphi(X,t)$ following the tip Z(t); by the chain rule,

$$\varphi^{\circ} = \varphi^{\circ} + \nabla \varphi \cdot \mathbf{v} \tag{2.11}$$

in bulk, where

$$\varphi^{\bullet}(\mathbf{X},t) = \partial \varphi(\mathbf{X},t) / \partial t.$$

We will repeatedly take limits, as $\delta \rightarrow 0$, of integrals over $\partial D_{\delta}(t)$ of fields of the form $\phi(\mathbf{X},t)\mathbf{n}(\mathbf{X},t)$, where, for example, ϕ is tensor-valued. We refer to such limits, when meaningful, as *tip integrals*, and write

$$\oint_{tip} \varphi n = \lim_{\delta \to 0} \int \varphi n.$$

The next definition allows us to state succintly our hypotheses concerning momenta and energies. We will refer to φ as *regular* if, in addition to being

smooth away from the tip,

- (1) φ is integrable on B; given any control volume R(t), the mapping t $\mapsto \int_{R(t)} \dot{\varphi}$ is differentiable;
- (2) φ° is integrable on B and $[\varphi]m \cdot v$ is integrable on C(t), both uniformly in t;
- (3) $\oint_{tip} \varphi n$ exists.

We will consistently use the following notation:

- $R_{\delta}(t) = R(t) \setminus D_{\delta}(t), \qquad (2.12a)$
- $\mathbf{\tilde{C}}_{\mathsf{R}}(\mathsf{t}) = \mathbf{\tilde{C}}(\mathsf{t}) \cap \mathsf{R}(\mathsf{t}), \tag{2.12b}$

$$C_{\delta}(t) = C_{D_{\delta}}(t) = C(t) \cap D_{\delta}(t) \qquad \text{for a tip disc,} \qquad (2.12c)$$

$$C_{\delta}(t) = C_{P_{\delta}}(t) = C(t) \cap P_{\delta}(t)$$
 for a pillbox. (2.12d)

Transport Theorems.

(i) Let R(t) be a control volume that does not contain the tip. If $\varphi(X,t)$ is smooth away from the tip, then

(ii) Let R(t) be a tip control-volume. If $\varphi(X,t)$ is regular, then

with $\int_{R(t)} \phi^*$ defined as $\lim_{\delta \to 0} \int_{R_\delta} \phi^*$, which exists. Furthermore,

The result (2.13) is standard, while proofs of (2.14) and (2.15) may be found in (1996, p. 913). Three additional results, each useful, are

$$\int \phi^* \to 0, \qquad (2.16a)$$
 D₈(t)

$$\int \varphi U_{\partial R} - (d/dt) \{ \int \varphi \} \rightarrow \oint_{tip} \varphi(\mathbf{v} \cdot \mathbf{n}),$$

$$\partial D_{\delta}(t) \qquad D_{\delta}(t)$$

$$(2.16b)$$

as $\delta \rightarrow 0$; (2.16a) follows from the existence of $\lim_{\delta \rightarrow 0} \int_{R_{\delta}} \varphi^*$; (2.16b) is a consequence of (2.15) and the first of (2.6); (2.16c) follows from (2.13) and the properties (i) and (ii) of the pillbox $P_{\delta}(t)$ defined in (2.8).

We now state two useful transport relations for fields $\delta(s)$ (independent of t) that are continuous on the crack. Using the notation of the paragraph containing (2.3), let

$$\delta_{tip}(t) = \delta(s(Z(t))), \quad \delta^{-}(t) = \delta(s(X^{-}(t)))$$
 for a tip control volume, (2.17a)
 $\delta^{\pm}(t) = \delta(s(X^{\pm}(t)))$ for a crack control volume; (2.17b)

then

$ (d/dt) \{ \int \delta \} = \delta_{tip} \nabla - \delta^{-} u^{-} \\ $	for a tip control volume,	(2.18a)
$ (d/dt) \left\{ \int \delta \right\} = \delta^{+}u^{+} - \delta^{-}u^{-} \\ $	for a crack control volume.	(2.18b)

Thus, by (2.7), as $\delta \rightarrow 0$,

3. MOTIONS

Let y(X,t) be a motion of B; that is, let y(X,t) be smooth away from the tip with y(X,t) one-to-one and bounded in X on B for each t. The deformation gradient

 $\mathbf{F} = \nabla \mathbf{y} \tag{3.1}$

and the material velocity \mathbf{y}^* are then smooth away from the tip.

Let R(t) be a control volume. The boundary curve $\partial R(t)$ may be parametrized in a sufficiently small time interval and in a neighborhood of any of its points by a function of the form $X = \hat{X}(\lambda, t)$ (λ a scalar variable); the field

$$\mathbf{u}(\mathbf{X},t) = \partial \hat{\mathbf{X}}(\lambda,t) / \partial t$$
(3.2)

then represents a velocity field for $\partial R(t)$ in that neighborhood. It is possible to use such parametrizations to construct a smooth velocity field u(X,t) for all of $\partial R(t)$ in any (sufficiently small) time interval. A field u so constructed depends on the choice of local parametrizations, but its normal component is intrinsic:

 $\mathbf{u} \cdot \mathbf{n} = \mathbf{U}_{\partial \mathbf{R}}. \tag{3.3}$

Each local parametrization $\mathbf{X} = \hat{\mathbf{X}}(\lambda, t)$ induces a corresponding local parametrization $\mathbf{x} = \hat{\mathbf{x}}(\lambda, t) = \mathbf{y}(\hat{\mathbf{X}}(\lambda, t), t)$ for the deformed boundary curve $\mathbf{y}(\partial \mathbf{R}(t), t)$; the corresponding *induced velocity field*

$$\overline{\mathbf{u}}(\mathbf{X},t) = \partial \widehat{\mathbf{x}}(\lambda,t) / \partial t \qquad (3.4)$$

for the deformed boundary $\mathbf{y}(\partial R(t),t)$ is related to u by the formula

$$\overline{\mathbf{u}} = \mathbf{y}^* + \mathbf{F}\mathbf{u}. \tag{3.5}$$

An intrinsic choice for \mathbf{u} is normal to ∂R ; in this case,

$$\mathbf{u} = U_{\partial R} \mathbf{n}, \qquad \mathbf{\bar{u}} = \mathbf{y}^* + U_{\partial R} \mathbf{F} \mathbf{n}.$$
 (3.6)

The tip velocity $\mathbf{v}(t)$ may be considered as a velocity field for the boundary of the disc $D_{\delta}(t)$ using as a parametrization

$$\mathbf{X} = \mathbf{X}_{\delta}(\lambda, t) = \mathbf{Z}(t) + \delta \boldsymbol{\nu}(\lambda),$$

with $\boldsymbol{\nu}(\lambda)$ a unit vector at an angle λ from a fixed axis. Then

$$\mathbf{y}^{\circ} = \mathbf{y}^{\bullet} + \mathbf{F}\mathbf{v} \tag{3.7}$$

represents the corresponding induced velocity field for $\mathbf{y}(\partial D_{\delta}(t),t)$. We assume there is a function $\mathbf{\bar{v}}(t)$ such that

$$\mathbf{y}^{\circ}(\mathbf{X},t) \rightarrow \overline{\mathbf{v}}(t)$$
 as $\mathbf{X} \rightarrow \mathbf{Z}(t)$, uniformly in (\mathbf{X},t) . (3.8)

If y(X,t) has a limiting value y(Z(t),t) as $X \to Z(t)$, so that the *deformed crack tip* is well defined, then y(Z(t),t) is differentiable in t and

$$\overline{\mathbf{v}}(t) = d\mathbf{y}(\mathbf{Z}(t), t)/dt. \tag{3.9}$$

A direct consequence of (3.7) and (3.8) is that

for
$$\mathbf{v} = \mathbf{0}$$
, $\mathbf{y}^{*}(\mathbf{X},t) \rightarrow \mathbf{\bar{v}}(t)$ as $\mathbf{X} \rightarrow \mathbf{Z}(t)$, uniformly in (\mathbf{X},t) . (3.10)

PART I. BALANCE LAWS FOR STANDARD AND CONFIGURATIONAL FORCES. SECOND LAW

4. FORCES

We consider two systems of forces: a standard system consistent with balance laws for linear and angular momentum; and a configurational system, consistent with its pecular balance, that maintains the structural integrity of the material.

a. Standard forces

We let S(X,t) denote the (Piola) stress that arises in response to deformation, let b(X,t) denote the inertial body force distributed over B, consider an inertial body force i(t) concentrated at the tip, and neglect all other external body forces. We assume that S is smooth away from the tip; that the crack faces are traction-free:

$$\lim_{\varepsilon \to 0} S(X \pm \varepsilon m(X), t)m(X) = 0 \quad \text{on } C(t);$$
(4.1)

that

$$\int |\mathbf{Sn}| \quad \text{is bounded as } \delta \to 0; \tag{4.2}$$

$$\partial D_{\delta}(t)$$

and that **b** is integrable over B. The standard balance laws for forces and moments then take the following form for each of the three types of control volumes R=R(t):

 $\int \mathbf{Sn} + \int \mathbf{b} = \mathbf{0}, \qquad \int \mathbf{y} \times \mathbf{Sn} + \int \mathbf{y} \times \mathbf{b} = \mathbf{0} \quad (\text{bulk or crack control-volume}), \quad (4.3a)$ $\partial \mathbf{R} \quad \mathbf{R} \qquad \partial \mathbf{R} \quad \mathbf{R} \qquad \qquad \\ \int \mathbf{Sn} + \int \mathbf{b} + \mathbf{i} = \mathbf{0}, \qquad \int \mathbf{y} \times \mathbf{Sn} + \int \mathbf{y} \times \mathbf{b} + \mathbf{y} \times \mathbf{i} = \mathbf{0} \qquad (\text{tip control-volume}), \quad (4.3b)$ $\partial \mathbf{R} \quad \mathbf{R} \qquad \qquad \partial \mathbf{R} \quad \mathbf{R} \qquad \qquad$

with $y \times i = y(Z(t),t) \times i(t)$. The balances (4.3a) are together equivalent to the local relations

$$\operatorname{div} \mathbf{S} + \mathbf{b} = \mathbf{0}, \qquad \mathbf{S} \mathbf{F}^{\mathsf{T}} = \mathbf{F} \mathbf{S}^{\mathsf{T}}$$
(4.4)

in bulk. Further, since **b** is integrable and **y** bounded, (4.3b) applied to a tip disc

 $D_{\delta}(t)$ yields, in the limit $\delta \rightarrow 0$, the following balances at the tip:

$$\oint_{tip} Sn + i = 0, \qquad \oint_{tip} y \times Sn + y \times i = 0.$$
(4.5)

b. Configurational forces

We consider a configurational force system consisting of a stress tensor C(X,t), a body force d(X,t) distributed over B, a force h(X,t) distributed over the crack C(t), a force g(t) concentrated at the tip, and a surface stress vector $\sigma(s)$ that acts within the free surfaces of the crack (Figure 3).¹¹

The force **g** is a sum

$$\mathbf{g} = \mathbf{g}_{\text{ext}} + \mathbf{g}_{\text{int}}, \tag{4.6}$$

with \mathbf{g}_{ext} inertial and \mathbf{g}_{int} an internal force that maintains the integrity of the tip when the crack is stationary and acts in response to the breaking of bonds during propagation. The forces **d** and **h** also have inertial and internal components, but the corresponding decompositions are irrelevant to what follows.¹²

Fix s and t, and let $\mathbb{C}^+ = \mathbb{C}^+(t)$ {respectively, $\mathbb{C}^- = \mathbb{C}^-(t)$ } denote the portion of the crack with arc-length values greater than {respectively, less than} s. The surface stress $\sigma = \sigma(s)$ then represents the force exerted across s by the material in \mathbb{C}^+ on the material in \mathbb{C}^- , with $\sigma \cdot \mathbf{e}$ a surface tension and $\sigma \cdot \mathbf{m}$ a surface shear. (Here the term "material" signifies the material of both crack faces.)

We assume that C is smooth away from the tip, that d is integrable on B, and that h is integrable and σ continuous on C(t). We posit a *configurational* force balance that has the following form for each of the three types of control

 1^{2} Internal body forces have no classical counterpart. A choice of reference configuration is an identification of the body's material points with points of euclidean space. Internal forces represent forces that pin these reference labels in place (GURTIN 1995,1997). An operational view of such forces may be phrased in terms of an underlying lattice. A choice of reference pins this lattice to the underlying ambient space. If the material undergoes fracture, then the lattice, in the reference, remains unchanged, but since bonds between atoms have been broken, additional internal forces are needed to preserve the referential integrity of the lattice. At the tip such forces are represented by g_{int} , a quantity that will be central to the constitutive description of tip kinetics (1996).

¹¹We allow neither σ nor the surface energy ψ (cf. §5a) to depend on t. Such dependences, while not difficult to accomodate, seem unimportant to the characterization of real materials, for which σ and ψ typically depend constitutively on the normal **m** to C, while $\mathbf{m} = \mathbf{m}$ (s) is independent of t (cf. HERRING 1951a, HOFFMAN and CAHN 1972). One generally expects a configurational shear $\sigma \cdot \mathbf{m}$ whenever the surface energy is constitutively anisotropic (cf., HERRING 1951a, HOFFMAN and CAHN 1972).



Figure 3 Configurational forces acting on a control volume R.

volumes R=R(t) (cf. (2.12b), (2.17)):

$$\int \mathbf{Cn} + \int \mathbf{d} = \mathbf{0} \qquad (bulk \text{ control-volume}), \qquad (4.7a)$$

$$\partial \mathbf{R} \quad \mathbf{R} \qquad \int \mathbf{Cn} + \int \mathbf{d} + \int \mathbf{h} + \mathbf{\sigma}^{+} - \mathbf{\sigma}^{-} = \mathbf{0} \qquad (crack \text{ control-volume}), \qquad (4.7b)$$

$$\partial \mathbf{R} \quad \mathbf{R} \quad \mathbf{C}_{\mathbf{R}} \qquad \qquad (tip \text{ control-volume}). \qquad (4.7c)$$

$$\partial \mathbf{R} \quad \mathbf{R} \quad \mathbf{C}_{\mathbf{R}} \qquad \qquad (tip \text{ control-volume}). \qquad (4.7c)$$

The balance (4.7a) yields the relation

$$\operatorname{div} \mathbf{C} + \mathbf{d} = \mathbf{0} \tag{4.8}$$

in bulk.

To derive a local relation for the crack, consider an arbitrary pillbox $P_{\delta}(t)$. Then (4.7b) applied to $P_{\delta}(t)$ yields, in the limit $\delta \rightarrow 0$,

 $\int_{s^{-}}^{s^{+}} ([C]m + h) + \sigma^{+} - \sigma^{-} = 0,$

where $s^{\pm}=s^{\pm}(t)$, $s^{+}>s^{-}$, are the arc lengths values that mark the endpoints of $P_{\delta}(t)$, while $\sigma^{\pm} = \sigma(s^{\pm})$. If we let $s^{+} \rightarrow s^{-}$ after dividing by $s^{+} - s^{-}$, we find that

$$[C]m + h + d\sigma/ds = 0 \tag{4.9}$$

on the crack away from the tip.

Finally, since **d** and **h** are integrable, (4.7c) applied to a tip disc $D_{\delta}(t)$ yields, in the limit $\delta \rightarrow 0$, the tip balance

$$\oint_{tip} Cn + g_{int} + g_{ext} - \sigma_{tip} = 0, \qquad \sigma_{tip} = \sigma(s(Z(t))), \qquad (4.10)$$

where we have used (4.6).

c. Inertial forces. Kinetic energy

Let $\rho(\mathbf{X}) \ge 0$ denote the mass density, assumed continuous, and write

$$\mathbf{k} = \frac{1}{2} \rho |\mathbf{y}^*|^2, \qquad \mathbf{p} = \rho \mathbf{y}^* \tag{4.11}$$

for the densities of momentum and kinetic energy. We define the production of momentum and kinetic energy in a control volume R(t) through

$$\mathbf{P}(\mathbf{R}(t)) = (d/dt) \{ \int \mathbf{p} \} - \int \mathbf{p} U_{\partial \mathbf{R}}, \qquad (4.12a)$$

R(t) $\partial \mathbf{R}(t)$

$$K(R(t)) = (d/dt) \{ \int k \} - \int k U_{\partial R},$$

R(t) $\partial R(t)$ (4.12b)

and, to ensure that these definitions have meaning, we assume that \mathbf{p} and \mathbf{k} are regular.

As in (1996) and in PODIO-GUIDUGLI (1996), we characterize inertial forces through the following two relations involving inertial forces, inertial working, and the productions of momentum and kinetic energy:

$$\int b + i = -P(R),$$
 (4.13a)
R

$$\int \mathbf{b} \cdot \mathbf{y}^* + \mathbf{i} \cdot \mathbf{\bar{v}} + \mathbf{g}_{ext} \cdot \mathbf{v} = -K(R).$$
(4.13b)
R

The relations (4.13) {respectively, (4.13) with the terms involving **i** and \mathbf{g}_{ext} omitted} are to be satisfied for each tip control volume {respectively, crack or bulk control volume} R=R(t). Here $\int_R \mathbf{b} \cdot \mathbf{y}^*$ denotes the limit $\lim_{\delta \to 0} \int_{R_{\delta}} \mathbf{b} \cdot \mathbf{y}^*$, which we assume to exist.

The counterpart of (4.13a) for bulk control volumes yields the standard result

$$\mathbf{b} = -\rho \mathbf{y}^{**}. \tag{4.14}$$

More important are the relations¹³

$$\mathbf{i} = \mathbf{\phi}_{\mathrm{tip}} \mathbf{p}(\mathbf{v} \cdot \mathbf{n}), \tag{4.15a}$$

$$\mathbf{i} \cdot \mathbf{\bar{v}} + \mathbf{g}_{ext} \cdot \mathbf{v} = \oint_{tip} k(\mathbf{v} \cdot \mathbf{n}), \qquad (4.15b)$$

$$\mathbf{g}_{\text{ext}} \cdot \mathbf{v} = \mathbf{v} \cdot \oint_{\text{tip}} k_{\text{rel}} \mathbf{n}, \qquad k_{\text{rel}} = \frac{1}{2} \rho |\mathbf{y}^* - \overline{\mathbf{v}}|^2; \qquad (4.15c)$$

(4.15a) asserts the equivalence of i and the release rate for momentum; (4.15b) ^{13}Cf . DASCALU and MAUGIN [1993], who, for a homogeneous elastic material, formally derive a relation (their eq. (6)) that implies (4.15c). DASCALU and MAUGIN base their result on a balance, analogous to (4.12a), for the "pseudomomentum" $\mathbf{p} = -p\mathbf{F}^{\mathsf{T}}\mathbf{y}^*$ (cf. MAUGIN 1993, 1995; GURTIN 1997); that balance yields a relation for \mathbf{g}_{ext} , rather than for $\mathbf{g}_{ext}^*\mathbf{v}$.

the equivalence of the total inertial-working and the release rate for kinetic energy; (4.15c) the equivalence of the configurational inertial-working and the release rate for the kinetic energy measured relative to the tip.

To establish (4.15), note first that, since \mathbf{b} and $\mathbf{b} \cdot \mathbf{y}^*$ are integrable,

$$\begin{array}{ccc} \int \mathbf{b} \to \mathbf{0}, & \int \mathbf{b} \cdot \mathbf{y}^* \to \mathbf{0} \\ D_{\delta} & D_{\delta} \end{array}$$
 (4.16)

as $\delta \rightarrow 0$. The identity (4.15a) follows from (2.16b), (4.12a), (4.13a), and the first of (4.16); (4.15b) follows from (2.16b), (4.12b), (4.13b), and the second of (4.16); (4.15c) follows from (4.15ab), the identity

$$\mathbf{k} - \mathbf{p} \cdot \mathbf{\bar{v}} = \frac{1}{2} \rho |\mathbf{y}^* - \mathbf{\bar{v}}|^2 - \frac{1}{2} \rho |\mathbf{\bar{v}}|^2, \tag{4.17}$$

and the continuity of ρ and spatial independence of $\bar{\mathbf{v}}$.

5. THE SECOND LAW

In the absence of thermal and compositional effects classical continuum mechanics may be based on a "second law" that utilizes *stationary* control volumes R and has the form

with $\Psi(X,t)$ the bulk free-energy. For a *migrating* control volume R=R(t) the standard generalization of this inequality would include the transport term

{inflow of free energy} =
$$\int \Psi U$$
 (5.1)
 ∂R

on the right side, but would not account for configurational forces.

We base the theory on what we believe to be a more fundamental version of the second law; specifically, we write the second law for a migrating control volume R=R(t) in a form

(d/dt){free energy of R(t)} \leq

{rate at which work is performed on R(t)}

that accounts for the working of both configurational forces and standard forces, but not explicitly for the flow (5.1) of free energy across R(t) as it migrates (GURTIN, 1995, eqt. (3.12)). (As we shall see, this inflow of free energy will be accounted for implicitly in the working of the configurational forces.)

a. Statement of the second law

We represent the free energy of the material by a bulk free-energy $\Psi(\mathbf{X},t)$ distributed over B and a surface free-energy $\psi(s)$ distributed over $\mathbb{C}(t)$; the free energy of R(t) is then given by

$$\int \Psi + \int \psi. \\ R(t) \quad C_{R}(t)$$

We assume that $\Psi(\mathbf{X},t)$ is regular and $\psi(s)$ smooth, that

ψ > Ο,

(5.2)

and that ψ is independent of time (*cf.* Footnote 11).

The working $\mathfrak{U}(R(t))$ should account for the work performed in the addition and removal of material at the boundary of R(t) and for the change in material structure as the crack tip evolves. We assume that $Cn \cdot u$ represents the boundary working of the configurational stress C, where u is the velocity field computed via a particular choice of local parametrizations $\mathbf{X} = \mathbf{\tilde{X}}(\lambda, t)$ for $\partial \mathbf{R}(t)$. Classically, the standard stress S expends power over the material velocity y^* , but when the control volume migrates there is no intrinsic material description of its deformed boundary $y(\partial R(t),t)$, as material is being added and removed, and it would seem appropriate to use, as a velocity for $y(\partial R(t),t)$, the derivative $\bar{u}(X,t)$ of $y(X(\lambda,t),t)$ with respect to t holding the surface parameter λ fixed (cf. (3.4)); we therefore write the boundary working of S in the form $Sn \cdot \bar{u}$.

The vector σ represents configurational stresses within the free surfaces of the crack. If R(t) is a crack (respectively, tip) control-volume, then σ performs work of amount $\sigma^{+}(X^{+})^{-} - \sigma^{-}(X^{-})^{+}$ {respectively, $-\sigma^{-}(X^{-})^{+}$ } (cf. (2.17) and the paragraph containing (2.3), (2.4)).

Since material is neither added nor removed from interior points of R(t), and since there is no change in material structure away from the crack tip, the working of the body force b should have its standard form b.y., while the configurational forces d and h should not perform work. Finally, the motion of the tip is accompanied by working of the inertial forces \mathbf{g}_{ext} and \mathbf{i} , with the tip velocities ${f v}$ and $ar{{f v}}$, respectively, as the appropriate conjugate velocities; on the other hand, the internal force \mathbf{g}_{int} , as such, performs no work.

In view of the foregoing discussion, we write the working $\mathfrak{V}(R(t))$ in the form

$$\begin{aligned}
\mathfrak{V}(R(t)) &= \int (\mathbf{Sn} \cdot \mathbf{\bar{u}} + \mathbf{Cn} \cdot \mathbf{u}) + \int \mathbf{b} \cdot \mathbf{y}^* + \mathfrak{V}_c(R(t)), \\ \partial R(t) & R(t) \end{aligned} \tag{5.3}$$

where $\mathfrak{W}_{c}(R(t))$, the working associated with the crack, has the following form for each of the three types of control volumes R=R(t) (cf. (2.3), (2.4), 2.20)):

$\mathfrak{W}_{c}(\mathbf{R}) = 0$	(bulk control-volume),	(5.4a)	
Ψ _c (R) = u* e*·σ * - u ⁻ e ⁻ ·σ ⁻	(crack control-volume),	(5.4b)	

 $\mathfrak{W}_{c}(\mathbf{R}) = \mathbf{i} \cdot \mathbf{\overline{v}} + \mathbf{g}_{ext} \cdot \mathbf{v} - \mathbf{u}^{-} \mathbf{e}^{-} \cdot \boldsymbol{\sigma}^{-}$ (tip control-volume). (5.4c)

We therefore write the second law for a control volume R(t) — that may or may not contain the crack tip — in the form

with **u** a velocity field for $\partial R(t)$ and $\overline{\mathbf{u}}$ the corresponding induced velocity field for $\mathbf{y}(\partial R(t),t)$. The quantity

$$\Gamma(\mathbf{R}) := \int (\mathbf{Sn} \cdot \bar{\mathbf{u}} + \mathbf{Cn} \cdot \mathbf{u}) + \int \mathbf{b} \cdot \mathbf{y}^* + \mathcal{W}_c(\mathbf{R}) - (d/dt) \{ \int \Psi + \int \psi \} \ge 0 \quad (5.6)$$

$$\partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{C}_{\mathbf{R}}$$

represents the energy dissipated in R=R(t), per unit time.

b. The second law applied to bulk and crack control-volumes

We require that the second law (5.5) be independent of the choice of parametrization for $\partial R(t)$. A consequence of this requirement, applied to an arbitrary timedependent bulk control-volume, is the *Eshelby relation*

$$\mathbf{C} = \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \tag{5.7}$$

for the configurational stress (GURTIN, 1995). Using (3.3), (3.5), and (5.7), we can rewrite (5.5) in the more familiar form

when applied to an arbitrary, time-independent, bulk control-volume, (5.8) yields the bulk dissipation inequality $\Psi^* \leq \mathbf{S} \cdot \mathbf{F}^*$.

Consider next a pillbox $P_{\delta}=P_{\delta}(t)$. Since $P_{\delta}(t)$ does not contain the tip, and since ψ is independent of time, (2.16c), (2.18b), the assertions (i) and (ii) following (2.8), (4.1), and (5.4b) imply that

 $\begin{aligned} (d/dt) \{ \int \Psi + \int \psi \} &\to \psi^+ u^+ - \psi^- u^-, \\ & P_\delta \quad \overline{C}_\delta \\ \\ \int (\mathbf{Sn} \cdot \mathbf{y}^* + \Psi U_{\partial R}) + \int \mathbf{b} \cdot \mathbf{y}^* &\to 0, \\ \partial P_\delta & P_\delta \\ \\ \Psi (P_\delta) &\to u^+ \mathbf{e}^+ \cdot \sigma^+ - u^- \mathbf{e}^- \cdot \sigma^-, \end{aligned}$

as $\delta \rightarrow 0$. Thus (5.8) yields

and since u^{\pm} may be specified arbitrarily, we arrive at the equivalence of surface tension and surface free energy,

$$\boldsymbol{\sigma} \boldsymbol{\cdot} \boldsymbol{e} = \boldsymbol{\psi}. \tag{5.10}$$

c. The second law applied to tip control-volumes

Consider (5.5) applied to the tip disc $D_{\delta}=D_{\delta}(t)$. By (2.15) and (2.19),

$$\begin{array}{ccc} (d/dt) \{ \int \Psi + \int \psi \} \rightarrow 0 \\ D_{\delta} & \mathbb{C}_{\delta} \end{array}$$

as $\delta \rightarrow 0$; thus, appealing to the paragraph containing (3.7), we conclude, with the aid of (4.16), (5.4c), and (5.6) that

$$\int (\mathbf{Sn} \cdot \mathbf{y}^\circ + \mathbf{Cn} \cdot \mathbf{v}) + \mathbf{i} \cdot \mathbf{\bar{v}} + \mathbf{g}_{ext} \cdot \mathbf{v} - \mathbf{u}^- \mathbf{e}^- \cdot \boldsymbol{\sigma}^- + o(1) = \Gamma(\mathbf{D}_{\delta}) \ge 0.$$
(5.11)
$$\partial \mathbf{D}_{\delta}$$

Next, by (3.8), (4.2), and the first of (4.5), as $\delta \rightarrow 0$,

$$\int \mathbf{Sn} \cdot \mathbf{y}^{\circ} = \mathbf{\bar{v}} \cdot \int \mathbf{Sn} + o(1) \rightarrow -\mathbf{\bar{v}} \cdot \mathbf{i},$$

$$\partial D_{\delta} \qquad \partial D_{\delta}$$
(5.12)

while (4.10) yields

$$\int \mathbf{Cn} \cdot \mathbf{v} = \mathbf{v} \cdot \int \mathbf{Cn} \to \mathbf{v} \cdot (\boldsymbol{\sigma}_{tip} - \mathbf{g}_{int} - \mathbf{g}_{ext}).$$
(5.13)
$$\partial D_{\delta} \qquad \partial D_{\delta}$$

Thus, by (2.2) and (2.7), passing to the limit $\delta \rightarrow 0$ in (5.11) yields two important results:

$$\mathbf{g}_{\text{int}} \cdot \mathbf{v} \le \mathbf{0}, \tag{5.14}$$

which represents an internal dissipation inequality for the crack tip; and

$$\Gamma_{\rm tip} = -\mathbf{g}_{\rm int} \cdot \mathbf{v}, \qquad \Gamma_{\rm tip} = \lim_{\delta \to 0} \Gamma(D_{\delta}), \qquad (5.15)$$

establishing $-g_{int}$, and hence the breaking of bonds, as the sole source of dissipation at the tip.

By (4.12b), (4.13b), (5.4c) and (5.10), we can write the second law (5.8) for a tip control-volume R=R(t) in the form

and can express $\Gamma(R)$, defined by (5.6), as the right side of (5.16) minus the left. Since $\int_{\partial R} (\Psi + k) U_{\partial R}$ and $-\psi^- u^-$, respectively, represent net flows of bulk and surface energy into R across ∂R , (5.16) is consistent with more standard views concerning the formulation of basic laws for control volumes. (For a crack control-volume there would be an additional term $\psi^+ u^+$ on the right side of (5.16); for a bulk control-volume the terms involving ψ would be omitted.)

In view of the sentence containing (5.16), we find, with the aid of (2.15) and (2.19), that

$$\oint_{tip} \{ \mathbf{Sn} \cdot \mathbf{y}^* + (\Psi + \mathbf{k}) (\mathbf{v} \cdot \mathbf{n}) \} - \psi_{tip} \mathbf{V} = \Gamma_{tip}, \qquad (5.17)$$

which can be regarded as an energy balance for the crack tip.

6. BASIC DEFINITIONS AND RESULTS FOR THE CRACK TIP

a. Tip traction. Tip J-integral. Driving force

Let e(t) = e(Z(t)). The following quantities are essential to our discussion:

$$\mathbf{j} := \oint_{\text{tip}} \{ (\Psi + \mathbf{k}_{rel}) \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n} \qquad tip \ traction, \qquad (6.1a)$$

$$J := \mathbf{e} \cdot \mathbf{j} = \mathbf{e} \cdot \mathbf{j}_{tip} \{ (\Psi + \mathbf{k}_{rel}) \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n} \qquad energy \ release \ rate, \qquad (6.1b)$$

$$f := J - \psi_{tip}$$
 driving force. (6.1c)

The vector **j** represents the configurational traction $\oint_{tip} Cn$ on the material in an infinitesimal neighborhood of the tip, augmented by the "inertial traction" $\oint_{tip} k_{rel}n$.

With a view toward discussing f and J, we assume throughout the remainder of this subsection that the crack is growing:

$$\mathbf{v} = \mathbf{V}\mathbf{e}, \qquad \mathbf{V} > \mathbf{0}.$$
 (6.2)

Since $\mathbf{e} \cdot \boldsymbol{\sigma}_{tip} = \psi_{tip}$, (4.15c), divided by V, and (6.1c) imply that

$$\mathbf{f} = \mathbf{e} \cdot \left[\oint_{\text{tip}} \{ \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n} - \sigma_{\text{tip}} + \mathbf{g}_{\text{ext}} \right].$$
(6.3)

The stress $\mathbf{C} = \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S}$, the surface stress $\boldsymbol{\sigma}$, and the inertial force \mathbf{g}_{ext} give rise to a net *non-internal* configurational force on the material in an infinitesimal neighborhood of the tip; f represents the component of that force in the direction of propagation. Using the Eshelby relation (5.7), we can rewrite the configurational balance (4.10) in the form

$$\oint_{\text{tip}} \{\Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S}\} \mathbf{n} - \sigma_{\text{tip}} + \mathbf{g}_{\text{int}} + \mathbf{g}_{\text{ext}} = \mathbf{0}.$$
(6.4)

The last two relations yield the tangential configurational balance

$$\mathbf{f} = -\mathbf{e} \cdot \mathbf{g}_{\text{int}}, \tag{6.5}$$

a balance between the driving force f and $-e \cdot g_{int}$, the internal force that opposes motion of the tip (*cf.* (1.1)). By (5.14) and (5.15),

$$\Gamma_{\rm tip} = fV \ge 0, \tag{6.6}$$

and hence the driving force f is work-conjugate to the tip speed V.

Letting $f = \Gamma_{tip}/V$, with Γ_{tip} given by (5.17), and comparing the result to (6.2), we conclude, with the aid of (6.1c), that

$$J = V^{-1} \oint_{tip} \{ \mathbf{Sn} \cdot \mathbf{y}^* + (\Psi + \mathbf{k}) (\mathbf{v} \cdot \mathbf{n}) \};$$
(6.7)

JV therefore represents the working on—and bulk-energy flow into—an infinitesimal neighborhood of the tip; J itself measures this quantity per unit cracklength rather than per unit time. Also, by (6.1b), J is the component of j in the direction of propagation; for $k_{rel} = 0$, J is the limiting value of the Eshelby-Rice integral.

Consequences of the tangential balance (6.5) and the second law, as manifested by the internal dissipation inequality (5.14), are the following necessary conditions for crack growth:

(i) the driving force must be nonnegative,

$$f \ge 0;$$
 (6.8)

(ii) the tip traction must form an acute angle with the direction of propagation,

$$\mathbf{e} \cdot \mathbf{j} \ge \psi_{\mathrm{tip}} > \mathbf{0}. \tag{6.9}$$

The Griffith criterion asserts that a crack will run when and only when $\mathbf{e} \cdot \mathbf{j} > \psi_{tip}$ and hence whenever (6.8) is satisfied strictly. Within the present framework (6.8) represents only a necessary condition for crack propagation; in fact for the class of constitutive equations we will consider, (6.8) may be satisfied strictly without motion of the tip. The results (6.8) and (6.9) are, however, independent of constitutive assumptions.

b. Summary of basic equations

The basic equations for the crack tip consist of the standard *force and moment* balances

$$\oint_{\text{tip}} \mathbf{Sn} + \mathbf{i} = \mathbf{0}, \qquad \oint_{\text{tip}} (\mathbf{y} \times \mathbf{Sn}) + \mathbf{y} \times \mathbf{i} = \mathbf{0}, \qquad (6.10)$$

and the tangential configurational balance

$$\mathbf{f} + \mathbf{e} \cdot \mathbf{g}_{\text{int}} = \mathbf{0} \tag{6.11}$$

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(cf. (6.5)). These balances are supplemented by a relation

$$\boldsymbol{e} \cdot \boldsymbol{\sigma}_{\mathrm{tip}} = \boldsymbol{\psi}_{\mathrm{tip}} > 0 \tag{6.12}$$

establishing the equivalence of surface tension and surface free energy (*cf.* (5.10)), and an *internal dissipation inequality*

$$e \cdot g_{int} \le 0 \quad \text{for V} > 0,$$
 (6.13)

which is the second law localized to the crack tip (cf. (5.14)); in this regard,

$$\Gamma_{\rm tip} = -(\mathbf{e} \cdot \mathbf{g}_{\rm int}) \mathbf{V} = \mathbf{f} \mathbf{V} \tag{6.14}$$

represents the energy dissipated at the tip, per unit time.

Remarks.

1. The surface shear $\mathbf{m} \cdot \mathbf{\sigma}$ and the normal internal force $\mathbf{m} \cdot \mathbf{g}_{int}$ perform no work, as there is no motion of the crack normal to itself; and the internal configurational forces **d** and **h** perform no work, since structural changes in the material occur only at the tip. For that reason, we consider these forces as *indeterminate*¹⁴ and view the balances (4.8), (4.9), and the normal part of (6.4) as equations for **d**, **h**, and $\mathbf{m} \cdot (\mathbf{\sigma} + \mathbf{g}_{int})$.¹⁵ On the other hand, the surface tension $\mathbf{e} \cdot \mathbf{\sigma}$ and the tangential force $\mathbf{e} \cdot \mathbf{g}_{int}$ perform work, but only when the crack tip advances. Configurational forces therefore play no role away from the tip,¹⁶ while at the tip the sole operative forces are those involved in the tangential part of the balance (6.4), namely J, $\mathbf{e} \cdot \mathbf{\sigma}_{tip} = \psi_{tip}$, and $\mathbf{e} \cdot \mathbf{g}_{int}$ (cf. (6.1c), (6.5)). Bulk constitutive equations for **4** and **5** yield, via (6.1b), an auxiliary constitutive specification for J; in the next section we will discuss constitutive equations for both ψ_{tip} and the internal force $\mathbf{e} \cdot \mathbf{g}_{int}$.

2. It is important to differentiate between the roles played by the surface energy

¹⁴That is, not specified constitutively (TRUESDELL and NOLL, 1965, p. 70).

¹⁵Contrast this to a phase interface, whose migration results in the working of internal configurational forces distributed over it and surface stresses acting within it. For that reason such forces are not treated as indeterminate; in fact, their constitution helps to characterize the kinetics of the interface (GURTIN and STRUTHERS, 1990; GURTIN 1995).

¹⁶The theory away from the tip is therefore equivalent to the classical theory. On the other hand, configurational forces play a pivotal role in the evolution of the tip, as it is there that the material structure undergoes change.

 Ψ_{tip} , the energy release-rate J, and the tangential component $\mathbf{e} \cdot \mathbf{g}_{int}$ of the internal configurational force. Throughout the literature one finds constitutive prescriptions for J (or equivalently for the stress intensity factor). Our view is that $\mathbf{e} \cdot \mathbf{g}_{int}$ and Ψ_{tip} are constitutive, with J a defined quantity related to $\mathbf{e} \cdot \mathbf{g}_{int}$ and Ψ_{tip} through the tangential configurational balance (1.1). J is typically represented by bulk quantities that already have constitutive prescriptions (cf. Remark 1); to write an additional constitutive equation for J would seem inappropriate. In the theory described here the configurational force balance provides a quantity \mathbf{g}_{int} with tangential component available for constitutive prescription. The physical consistency of this view is underlined by the fact that the second law yields the single inequality $\Gamma_{tip} = -\mathbf{V}\mathbf{e} \cdot \mathbf{g}_{int} \leq 0$, involving the same variable, whose satisfaction indicates the need for additional constitutive assumptions involving V and $\mathbf{e} \cdot \mathbf{g}_{int}$. In short, our view is that the prescription of a constitutive equation for J masks:

(i) the presence of a fundamental balance law, the configurational force balance;

(ii) the existence of a physically significant quantity, the internal configurational force, which acts at the tip, with tangential component $\mathbf{e} \cdot \mathbf{g}_{int}$ a direct response to the breaking of bonds during fracture. \Box

e. The standard momentum-condition

The quantity $\mathbf{i} = \oint_{tip} \mathbf{p}(\mathbf{v} \cdot \mathbf{n}) = [\oint_{tip} \mathbf{p} \otimes \mathbf{n}] \mathbf{v}$ represents the momentum flow into an infinitesimal neighborhood of the crack tip. Theories of crack propagation for specific materials are generally consistent with the hypothesis

$$\oint_{\text{tip}} \mathbf{p} \otimes \mathbf{n} = \mathbf{0} \tag{6.15}$$

(cf. Footnote 6), which we refer to as the standard momentum-condition. Granted (6.15), i=0, so that, by (6.10),

$$\oint_{\text{tip}} \mathbf{Sn} = \mathbf{0} \qquad \oint_{\text{tip}} \mathbf{y} \times \mathbf{Sn} = \mathbf{0}. \tag{6.16}$$

Further, by (6.15), $\oint_{tip} (\mathbf{p} \cdot \mathbf{\bar{v}}) \mathbf{n} = 0$; thus, since $k_{rel} = \frac{1}{2} \rho |\mathbf{y}^* - \mathbf{\bar{v}}|^2$ and $\mathbf{p} = \rho \mathbf{y}^*$,

$$\oint_{\text{tip}} k_{\text{rel}} n = \oint_{\text{tip}} kn. \tag{6.17}$$

The importance of (6.17) is that it results in relations

$$\mathbf{j} = \oint_{\text{tip}} \{ (\Psi + \mathbf{k}) \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}, \tag{6.18a}$$

$$J = \tau \cdot \mathbf{j} = \tau \cdot \mathbf{j}_{tip} \{ (\Psi + \mathbf{k})\mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}, \qquad (6.18b)$$

in which the tip traction \mathbf{j} does not depend explicitly on the speed or direction of the crack. (Without the standard momentum-condition \mathbf{j} is dependent on \mathbf{k}_{rel} and hence, by (3.7) and (3.8), on \mathbf{v} .)

By (3.10), for a stationary crack the standard momentum-condition is satisfied automatically; in fact, $\oint_{tip} kn = \oint_{tip} k_{rel}n = 0$, so that

$$\mathbf{j} = \oint_{\mathrm{tip}} \{ \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}, \qquad \mathbf{J} = \tau \cdot \oint_{\mathrm{tip}} \{ \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \} \mathbf{n}.$$
(6.19)

Throughout this part we assume that the standard momentum-condition is satisfied.

7. GROWING CRACKS

a. Constitutive relations at the tip

It is convenient to characterize the direction of propagation e by its counterclockwise angle θ from the (1,0) axis:

$$\mathbf{e} = \mathbf{e}(\mathbf{\theta}) = (\cos\mathbf{\theta}, \sin\mathbf{\theta}), \qquad \mathbf{m} = \mathbf{m}(\mathbf{\theta}) = (-\sin\mathbf{\theta}, \cos\mathbf{\theta}).$$
(7.1)

We consider two constitutive relations for the tip: one giving the surface energy ψ_{tip} as a function of θ ; the other giving the speed V as a function of θ and the component $-\mathbf{e} \cdot \mathbf{g}_{int}$ of the internal configurational force opposing propagation.

We write the constitutive equation for ψ_{tip} in the form

 $\psi_{tip} = \hat{\psi}(\Theta) \tag{7.2}$

with $\hat{\Psi}$ smooth and strictly positive:

 $\hat{\psi}(\theta) > 0. \tag{7.3}$

The force $-\mathbf{e} \cdot \mathbf{g}_{int}$ opposes the breaking of bonds at the tip, and it seems reasonable to suppose that propagation is possible only when this force is sufficiently large. For notational convenience, using the balance law (6.11), we write the constitutive equation for V in terms of θ and f, the driving force. We therefore consider, for the velocity V, a constitutive equation consisting of two parts: a fracture limit

$$V = 0 \qquad \text{for } f \le F(\theta), \qquad (7.4)$$

with

$$F(\theta) > 0 \tag{7.5}$$

the limit force for fracture; and a kinetic equation

$$V = \hat{V}(\theta, f) > 0 \qquad \text{for } f > F(\theta), \qquad (7.6)$$

with $\hat{V}(\theta, f)$ smooth up to $f = F(\theta)$ and consistent with $\lim_{f \to F(\theta)} \hat{V}(\theta, f) = 0$. The constitutive assumptions (7.4)-(7.6) ensure that $V \ge 0$, and, what is most important, that the dissipation inequality (6.6) be satisfied.

Remark. Materials scientists often model grain boundaries, phase boundaries, and free surfaces as sharp surfaces endowed with energy densities dependent on surface orientation (HERRING, 1951ab; FRANK, 1963; GJOSTEIN, 1963). In our theory surface physics of this type is characterized by the constitutive function $\hat{\psi}(\theta)$. In theories of phase boundaries such an energy $\hat{\psi}(\theta)$ gives rise to a vector surface stress of the form

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\psi}}(\boldsymbol{\theta})\boldsymbol{e}(\boldsymbol{\theta}) + \hat{\boldsymbol{\psi}}'(\boldsymbol{\theta})\mathbf{m}(\boldsymbol{\theta}), \tag{7.7}$$

where $\hat{\psi}(\theta)$ is surface tension, while $\hat{\psi}'(\theta)$ represents surface shear; moreover (7.7) follows from thermomechanical arguments (GURTIN, 1993, eqt. (6.12)). Here, unlike phase boundaries, the sole kinetics associated with the crack surfaces is that associated with the tip: the crack surface cannot move normal to itself. This "constraint" allows for $\boldsymbol{\sigma} \cdot \boldsymbol{e} = \hat{\psi}(\theta)$, but renders the surface shear $\boldsymbol{\sigma} \cdot \boldsymbol{m}$ indeterminate (cf. Remark 1 following (6.14)). \Box

b. Constitutively isotropic crack tips. Tips with constant mobility We will refer to the crack tip as *constitutively isotropic* if $\hat{\psi}(\theta)$, $\hat{V}(\theta,f)$, and $F(\theta)$ are independent of the orientation θ of the crack. Granted this, the constitutive equations (7.2)-(7.6) become

 $\psi_{tip} = \text{constant} > 0, \qquad (7.8a)$ $V = 0 \quad \text{for } f \le F, \qquad V = \hat{V}(f) > 0 \quad \text{for } f > F, \qquad (7.8b)$ $F = \text{constant} > 0, \qquad (7.8c)$

so that

 Φ = constant.

When considering such tips we will assume, in addition, that the speed increase with the driving force:

$$\hat{\mathbf{V}}'(\mathbf{f}) \ge 0 \quad \text{for } \mathbf{f} > \mathbf{F}.$$
 (7.9)

We will also consider *crack tips with constant mobility* as defined by the general anisotropic constitutive equations (7.2)-(7.6) with the kinetic relation (7.6) in the specific form

 $\hat{V}(\Theta, f) = M[f - F(\Theta)]$ for $f > F(\Theta)$, (7.10)

where

$$M > 0 \tag{7.11}$$

is a constitutive constant that represents the *mobility* of the crack tip.

c. The Griffith-Irwin function

We henceforth consider the energy release rate as a function

$$J(\Theta, \mathbf{j}) = \mathbf{e}(\Theta) \cdot \mathbf{j} \tag{7.12}$$

of the angle of propagation θ and the tip traction j. (When there is no danger of confusion we will suppress the argument j and write $J(\theta) = J(\theta, j)$.) For a material characterized by (7.2)-(7.6), crack propagation occurs when and only when $f > F(\theta)$, or equivalently, by (6.1c),

$$J(\theta,j) > \Phi(\theta),$$
 (7.13)

with

$$\Phi(\Theta) = \hat{\psi}(\Theta) + F(\Theta) > 0. \tag{1.2bis}$$

The Griffith criterion f>0 therefore represents a conservative estimate for propagation, at least within the present framework. We will refer to $\Phi(\theta)$ as the Griffith-Irwin function.¹⁷

 $^{^{17}}$ That surface energy is not the sole limiting factor to crack initiation was noted by IRWIN (1948), who proposed that ψ be augmented by a quantity δ_p representing the "plastic

d. Angle-convexity. The Frank diagram (GURTIN, 1993, §7)

Crack propagation is related to the convexity of the Griffith-Irwin function. The definition of convexity for such a function is not obvious: the usual definition is inapplicable, since $\Phi(\theta)$ is periodic.

A notion of convexity for $\Phi(\theta)$ can be given in terms of its *Frank diagram* Frank(Φ), which is the *curve* defined in polar coordinates (r, θ) by $r = \Phi(\theta)^{-1}$:

$$Frank(\Phi) = \{ (r, \theta) : r = \Phi(\theta)^{-1} \}$$
(7.14)

(FRANK, 1963). We will refer to $\Phi(\theta)$ as angle-convex if its Frank diagram is strictly convex; that is, if, given any angle α , the tangent to Frank(Φ) at the point **x** with angle α intersects Frank(Φ) only at **x**.

We will also consider nonconvex $\Phi(\theta)$; with this in mind, we will refer to a straight line \mathcal{L} as a *convexifying tangent* to Frank(Φ) if \mathcal{L} is tangent to Frank(Φ) at one or more points, but \mathcal{L} does not intersect the region interior to Frank(Φ); the angles of the points of intersection of \mathcal{L} with Frank(Φ) will then be referred to as *tangency angles* of \mathcal{L} (Figure 4).

Remarks.

1. An alternative but equivalent notion of convexity may be phrased in terms of the function $\tilde{\Phi}(\mathbf{x})$ defined for $|\mathbf{x}| \neq 0$ by

$$\widetilde{\Phi}(\mathbf{x}) = |\mathbf{x}|\Phi(\Theta), \tag{7.15}$$

with θ the angle of **x**, as the angle-convexity of $\Phi(\theta)$ is equivalent to the requirement that

$$\widetilde{\Phi}(\mathbf{x}) - \widetilde{\Phi}(\mathbf{z}) < (\mathbf{x} - \mathbf{z}) \cdot \nabla \widetilde{\Phi}(\mathbf{x})$$
(7.16)

for all non-zero points **x** and **z** whose angles are unequal. That angle-convexity should be related to the more standard convexity expressed by (7.16) becomes somewhat more transparent upon noting that, by (7.15), the level set $\tilde{\Phi}(\mathbf{x}) \equiv 1$ has the equation $\mathbf{r} = \Phi(\theta)^{-1}$.

2. For a further insight into the consequences of angle-convexity, let the energy of work dissipated in the surrounding material per unit surface area created" (cf. FREUND, 1990, pp. 8-10, from whom the quote is taken, and who gives a complete discussion of these ideas, with relevant references). Within our framework the role of y_p is played by F.



Figure 4 Frank diagram (the curve $Frank(\varphi)$) of a function $\varphi(\theta)$ that is not angleconvex. Σ is a convexifying tangent; θ_1 and θ_2 are tangency angles.

an oriented curve c be given by $\int_{C} E(\theta(s)) ds$, where $\theta(s)$ is the angle from a fixed axis to the unit tangent to c at s. Then $E(\theta)$ is angle-convex if and only if, among all oriented curves from one arbitrarily prescribed point to another, the straight line has (strictly) least energy.

3. The Wulff shape (or Wulff crystal) corresponding to $E(\theta)$ is the region W that minimizes $\int_{\partial U} E(\theta(s)) ds$ over the set of all regions W of unit area. The set of tangency angles of convexifying tangents to $E(\theta)$ then consists of the angles of all tangents to ∂W . (If $E(\theta)$ is not angle-convex, then ∂W will have corners, and some angles will be missing.) \Box

Lemma 7.1.

- (i) Strictly positive, constant functions are angle-convex. Thus for a constitutively isotropic tip, Φ is angle-convex.
- (ii) A necessary condition for the angle-convexity of $\Phi(\theta)$ is that

 $\Phi''(\theta) + \Phi(\theta) \ge 0 \tag{7.17}$

for all θ , where "primes" denote differentiation.

(iii) If $\hat{\psi}(\theta)$ and $F(\theta)$ are angle-convex, then so also is $\Phi(\theta)$.

Proof. Assertion (i) is immediate; (ii) is proved in (GURTIN, 1993, Theorem 7J); (iii) follows from the equivalence of angle-convexity and the condition expressed by (7.16).

We assume for the remainder of this section that a tip traction $\mathbf{j} \neq \mathbf{0}$ is prescribed and consider

 $J(\Theta) = J(\Theta, j)$

restricted to the set of angles θ with $\mathbf{e}(\theta) \cdot \mathbf{j} > 0$ (*cf.* (6.9), (7.12)). Then Frank(J) is the curve $\mathbf{r} = \{\mathbf{e}(\theta) \cdot \mathbf{j}\}^{-1}$; in fact, since $\mathbf{x} = \mathbf{r}\mathbf{e}(\theta)$,

Frank(J) is the straight line consisting of all \mathbf{x} such that $\mathbf{x} \cdot \mathbf{j} = 1$. (7.18)

A simple but important consequence of the notion of a Frank diagram is

Lemma 7.2. Given an angle θ ,

$$J(\theta) = \Phi(\theta) \iff \operatorname{Frank}(\Phi) \text{ intersects } \operatorname{Frank}(J)$$

at a point **x** with angle θ ; (7.19a)
$$J(\theta) < \Phi(\theta) \iff \text{ the point } \mathbf{x} \text{ on } \operatorname{Frank}(J) \text{ with angle } \theta$$

lies strictly outside of Frank(
$$\Phi$$
). (7.19b)

In the proof of the next lemma we will use the following consequences of (7.1):

$$\mathbf{e}'(\theta) = \mathbf{m}(\theta), \qquad \mathbf{m}'(\theta) = -\mathbf{e}(\theta).$$
 (7.20)

Lemma 7.3. Frank(J) is tangent to $Frank(\Phi)$ at a point with angle Θ_0 if and only if j satisfies

$$\mathbf{j} = \Phi(\Theta_0) \mathbf{e}(\Theta_0) + \Phi'(\Theta_0) \mathbf{m}(\Theta_0). \tag{7.21}$$

Proof. Assume that Frank(J) is tangent to Frank(Φ) at a point **x** with angle θ_0 . Then, by (7.19a), $J(\theta_0) = \mathbf{e}(\theta_0) \cdot \mathbf{j} = \Phi(\theta_0)$ holds. If we use (7.20) to differentiate, with respect to θ , the curves $r = \{\mathbf{e}(\theta) \cdot \mathbf{j}\}^{-1}$ and $r = \Phi(\theta)^{-1}$ representing Frank(J) and Frank(Φ), we see that these Frank diagrams are tangent at **x** if and only if

$$\mathbf{m}(\boldsymbol{\vartheta}_0) \cdot \mathbf{j} = \Phi'(\boldsymbol{\vartheta}_0). \tag{7.22}$$

The relations $\mathbf{e}(\theta_0) \cdot \mathbf{j} = \Phi(\theta_0)$ and (7.22) imply (7.21). Conversely, (7.21) implies $\mathbf{e}(\theta) \cdot \mathbf{j} = \Phi(\theta)$ and (7.22), and these yield the tangency of the Frank diagrams at \mathbf{x} .

8. KINKING AND CURVING OF CRACKS. MAXIMUM DISSIPATION CRITERION

In discussing kinks we will use local results derived for smooth cracks; this involves no inconsistencies, as these results will be applied only on the smooth portions of the crack.

Consider a stationary crack and a program of continuously increasing loads. Let θ^- denote the angle of the tangent $\mathbf{e}(\theta^-)$ at the tip. In certain circumstances one might expect crack propagation to initiate at an angle θ^+ different from θ^- , indicating an initial kink. Once the crack has begun to run, the surface energy and speed of the tip are given by (7.2) and (7.6) subject to (7.3) and (7.5); however an additional constitutive relation, specifying the direction of propagation, is needed. We derive this relation under the assumption that the crack will propagate in a direction that maximizes the rate at which it dissipates energy.

We will consistently use the following terminology: we begin with a stationary crack and use the term "crack initiation" to indicate the onset of a "running crack"; and to emphasize the possibility of kinking, we use the term "kink angle" for the angle θ^+ immediately after initiation, but in so doing we do not mean to rule out the case $\theta^+=\theta^-$.

We assume throughout this section that $e(\theta) \cdot j > 0$, an assumption involving no loss in generality (*cf.*, (6.9)).

a. Criterion for crack initiation. Kink angle

By (7.2) and (7.12), the driving force (6.1c) may be considered as a function of ϑ and the tip traction j:

$$\mathbf{f} = \mathbf{f}(\mathbf{j}, \mathbf{\Theta}) = \mathbf{J}(\mathbf{j}, \mathbf{\Theta}) - \hat{\boldsymbol{\psi}}(\mathbf{\Theta}), \tag{8.1}$$

We henceforth restrict attention to situations in which j is a continuous function of time at the instant of crack initiation,¹⁸ whether or not the crack develops an initial kink. This assumption renders the tip traction j a useful "parameter" for describing the loading in an arbitrarily small neighborhood of the crack tip. Also, since (7.4) and (7.6) are presumed to describe the dynamics of the crack, θ before initiation must be consistent with $J(j,\theta) \leq \Phi(\theta)$, while θ after initiation must satisfy $J(j,\theta) > \Phi(\theta)$. With this in mind, we refer to the tip traction j (or, more simply, to the loading) as:

(i) subcritical if $J(\mathbf{j}, \theta) < \Phi(\theta)$ for all θ ;

 $^{^{18}}$ We expect the continuity of **j**, at least when inertia is neglected.

- (ii) critical if $J(j,\theta) \leq \Phi(\theta)$ for all θ , but $J(j,\theta) = \Phi(\theta)$ for some θ (so that the loading is not subcritical);
- (iii) supercritical if, for some θ , $J(\mathbf{j},\theta) > \Phi(\theta)$.

Subcritical loading is then a necessary condition for a crack to remain stationary; supercritical loading is a necessary condition for crack propagatation; and critical loading is a necessary condition for crack initiation. The next theorem, a direct consequence of (7.19) and the foregoing definitions, shows the intimate relation between these conditions and the geometry of the Frank diagrams of J and Φ . In this regard, it should be noted that, by (7.18), there is a one-to-one correspondence between j and Frank(J).

Criticality Theorem. The tip traction j is:

(i) subcritical if and only if Frank(J) does not intersect $Frank(\Phi)$;

- (ii) critical if and only if Frank(J) is a convexifying tangent to $Frank(\Phi)$;
- (iii) supercritical if and only if Frank (J) intersects the region interior to $Frank(\Phi)$.

If the loading is critical, then those angles θ^+ that satisfy $J(\mathbf{j},\theta^+) = \Phi(\theta^+)$ will be referred to as *possible kink angles*, since, by (7.4) and (7.6), such angles mark the transition between $f < F(\theta)$ and $f > F(\theta)$ and hence between V = 0 and V > 0.

Initiation Theorem. Assume that the tip traction **j** is critical. Then, θ^+ is a possible kink angle if and only if θ^+ is a tangency angle of the convexifying tangent Frank(J) to Frank(Φ). Granted this, **j** is related to θ^+ through

$$\mathbf{j} = \Phi(\Theta^+) \mathbf{e}(\Theta^+) + \Phi'(\Theta^+) \mathbf{m}(\Theta^+). \tag{1.3bis}$$

Conversely, if for some convexifying tangent \mathcal{L} to $\Phi(\theta)$ and some tangency angle θ^+ of \mathcal{L} , (1.3) is satisfied, then j is critical.

Proof. Assume that j is critical. Then, the set of all possible kink angles θ^+ coincides with the set of θ^+ that satisfy $J(j,\theta^+) = \overline{\Phi}(\theta^+)$, we may use (ii) of the Criticality Theorem and (7.19a) to conclude that θ^+ is a possible kink angle if and only if θ^+ is a tangency angle of Frank(J). Granted this, (1.3) follows from Lemma 7.3.

Conversely, if for some convexifying tangent \mathcal{L} to $\operatorname{Frank}(\Phi)$ and some tangency angle θ^+ of \mathcal{L} , (1.3) is satisfied, then Lemma 7.3 (and the tacit smoothness of Φ) imply that $\mathcal{L} = \operatorname{Frank}(\Phi)$; the criticality of j then follows from (ii) of the Criticality Theorem. \Box **Corollaries.** Assume that **j** is critical.

(i) If $\Phi(\theta)$ is angle-convex, then there is at most one possible kink angle.

(ii) For a constitutively isotropic tip there is at most one kink angle θ^+ and, moreover,

$$\mathbf{e}(\mathbf{\Theta}^{+}) = \mathbf{j}/|\mathbf{j}|, \tag{8.2}$$

so that the direction of the kink coincides with the direction of \mathbf{j} . (iii) If the tip is constitutively anisotropic, and if θ^+ is a possible kink angle, then

$$\mathbf{m}(\mathbf{\Theta}^{+}) \cdot \mathbf{j}^{+} = \Phi'(\mathbf{\Theta}^{+}), \tag{8.3}$$

so that, for $\Phi'(\Theta^+) \neq 0$, **j** has a nonzero component normal to the direction of propagation corresponding to Θ^+ .

Proof. The result (i) is a consequence of the Initiation Theorem and the fact that for $\Phi(\theta)$ angle-convex, each tangent to $\operatorname{Frank}(\Phi)$ intersects $\operatorname{Frank}(\Phi)$ at exactly one point. For an isotropic tip Φ is constant and hence angle-convex, so that the kink angle is uniquely determined by **j**. Further, (1.3) with Φ = constant implies (8.2). For an anisotropic tip, (8.3) follows from (1.3). \Box

Remarks.

1. The formulas (7.7) for σ and (1.3) for j are identical granted the replacements

$$\sigma$$
 and $\hat{\psi}(\theta) \rightarrow j^{+}$ and $\Phi(\theta^{+})$. (8.4)

2. The results of this subsection give a geometric picture (Figure 5) of the qualitative aspects of the fracture process. A stationary crack will remain stationary as long as j is such that the line Frank(J) remains strictly outside the closed curve Frank(Φ). Initiation of a running crack begins at a time for which Frank(J) passes across Frank(Φ) with a portion of Frank(J) entering the open region Λ , say, interior to Frank(Φ), and the crack will continue to run as long as a portion of Frank(J) remains within Λ . At the time of initiation, Frank(J) touches Frank(Φ), but has no intersection with Λ ; hence Frank(J) must be a convexifying tangent, and the possible kink angles are those angles that mark the intersection of Frank(Φ) with Frank(J). \Box





Figure 5

Frank diagrams of $\overline{\Phi}$ and J: (a) for a stationary crack; (b) for possible initiation of a running crack (θ_1 and θ_2 are possible kink angles); (c) for a running crack (the angle describing the direction of propagation lies between θ_1 and θ_2).

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b. Maximum dissipation criterion for crack propagation

We now restrict attention to a running crack; by (7.6) and (8.1), this allows us to consider the dissipation rate (6.14) as a function of the tip traction j and the angle ϑ at which the crack advances:

$$\Gamma_{\rm tip} = \Gamma_{\rm tip}(j,\theta) = f \hat{V}(\theta,f), \qquad f = J(j,\theta) - \hat{\psi}(\theta), \qquad (8.5)$$

with j necessarily supercritical. A major hypothesis of our theory is that at each time t the angle $\theta = \theta(t)$ satisfy the maximum dissipation criterion:

$$\Gamma_{\rm tip}(j,\theta) = \max_{\alpha \in G(j)} \Gamma_{\rm tip}(j,\alpha), \tag{8.6a}$$

$$G(j) = \{ set of angles \theta such that J(j,\theta) > \Phi(\theta) \}.$$
(8.6b)

Then, since

the set $G(\mathbf{j})$ is a nonempty open set whose boundary consists of angles θ that satisfy $J(\mathbf{j}, \theta) = \Phi(\theta)$; furthermore,

$$\Gamma_{\rm tip}(\mathbf{j},\alpha) > 0$$
 for $\alpha \in \mathbf{G}(\mathbf{j})$, $\Gamma_{\rm tip}(\mathbf{j},\alpha) = 0$ for $\alpha \in \partial \mathbf{G}(\mathbf{j})$. (8.8)

Granted smoothness, the maximum problem (8.6) has a solution, and any such solution θ must satisfy

$$\partial \Gamma_{\rm tip}(\mathbf{j},\mathbf{\theta})/\partial\mathbf{\theta} = 0.$$
 (8.9)

It is important to note that the maximum dissipation criterion may not define a unique angle of propagation for a given value of j. The next lemma will be useful in determining conditions under which this angle is unique.

Lemma 8.1.

(i) Assume that $\Phi(\theta)$ is angle-convex. Then $G(\mathbf{j})$ is connected.

(ii) Assume that G(j) is connected. If

$$\partial^2 \Gamma_{\rm tip}(\mathbf{j}, \theta) / \partial \theta^2 < 0$$
 for all solutions $\theta \in \mathbb{G}(\mathbf{j})$ of (8.9), (8.10)

then (8.6) has a unique solution.

Proof. Let $J(\theta) = J(j,\theta) = j \cdot e(\theta)$. To establish (i) we must show that $\partial G(j)$ contains exactly two angles. $\partial G(j)$ consists of angles θ such $\Phi(\theta) = J(\theta)$; thus, by (7.19a), $\Omega := \operatorname{Frank}(\Phi) \cap \operatorname{Frank}(J)$ contains a point **x** for each such angle. Since $\Phi(\theta)$ is angleconvex, $\operatorname{Frank}(\Phi)$ is strictly convex; thus, since $\operatorname{Frank}(J)$ is a straight line, Ω contains at most two points, so that $\partial G(j)$ contains at most two angles. But G(j) is open; thus $\partial G(j)$ contains exactly two angles.

Assume that G(j) is connected. If $\Gamma_{tip}(j,\theta)$ were to have more than one maximum on G(j), then it would also have a minimum on G(j), and this would violate (8.10). Thus (ii) is valid. \Box

It is possible to obtain specific results for the direction of a running crack when the material is one of the specific types discussed in Subsection 7b. Here we continue to consider a running crack, so that the tip traction \mathbf{j} is necessarily supercritical.

Theorem on the Direction of a Running Crack.

 (i) For a constitutively isotropic tip the crack will propagate in the direction of the tip traction j:

$$\mathbf{e}(\mathbf{\Theta}) = \mathbf{j}/|\mathbf{j}|. \tag{8.11}$$

(ii) For a tip with constant mobility there is at least one angle θ at which the crack will propagate, and any such θ will satisfy the identity

$$\{2f(\theta, \mathbf{j}) - F(\theta)\}\{\mathbf{m}(\theta) \cdot \mathbf{j} - \hat{\psi}'(\theta)\} = f(\theta, \mathbf{j})F'(\theta).$$
(8.12)

If, in addition, Φ is angle-convex, then θ is unique.

Proof. We begin with some useful identities:

$$f(\mathbf{j}, \theta) = \mathbf{e}(\theta) \cdot \mathbf{j} - \hat{\psi}(\theta) > F(\theta) \ge 0 \quad \text{for all } \theta \in \mathbf{G}(\mathbf{j}), \quad (8.13a)$$

$$\mathbf{f}'(\mathbf{j},\mathbf{\Theta}) = \mathbf{m}(\mathbf{\Theta}) \cdot \mathbf{j} - \hat{\psi}'(\mathbf{\Theta}), \tag{8.13b}$$

$$\mathbf{f}''(\mathbf{j},\mathbf{\Theta}) = -\mathbf{e}(\mathbf{\Theta}) \cdot \mathbf{j} - \hat{\mathbf{\psi}}''(\mathbf{\Theta}), \qquad (8.13c)$$

where $f'(j,\theta) = \partial f(j,\theta) / \partial \theta$.

To establish (i) we set equal to zero the derivative of $\Gamma_{tip}(\theta) = f(\theta)\hat{V}(f(\theta))$; the

result is

$$f'\{\hat{V}'(f)f + \hat{V}(f)\} = 0. \tag{8.14}$$

Thus, assuming that the loading is supercritical, we may conclude from (8.13a), (7.8b), and (7.9) that the term $\{\cdots\}>0$, so that $f'(\theta) = 0$, which, by (8.13b) and the fact that $\hat{\psi}(\theta)$ is constant, yields

$$\mathbf{m}(\mathbf{\Theta}) \cdot \mathbf{j} = \mathbf{0}. \tag{8.15}$$

Also, since $f = e(\theta) \cdot j - \psi_{tip} > 0$, $e(\theta) \cdot j > 0$; thus (8.11) holds.

Consider (ii). Assume that the loading is supercritical. To establish the uniqueness of the angle of propagation, we fix j and write $f(\theta) = f(j,\theta)$ and $\delta(\theta) = \Gamma_{tip}(j,\theta)/M = f(\theta)[f(\theta) - F(\theta)]$; then

$$\delta' = f'(f - F) + f(f' - F'),$$
 (8.16a)

$$\mathbf{y}'' = \mathbf{f}''(\mathbf{f} - \mathbf{F}) + 2\mathbf{f}'(\mathbf{f}' - \mathbf{F}') + \mathbf{f}(\mathbf{f}'' - \mathbf{F}''). \tag{8.16b}$$

The formula (8.12) follows upon setting (8.16a) to zero, with the use of (8.13b). Assume that $\Phi(\theta)$ is angle-convex. Then (7.10), (7.17), (7.20), and (8.1) yield

 $f''+f=-\hat{\psi}''-\hat{\psi}, \qquad f''-F''+f-F=-\Phi''-\Phi\leq 0.$

Thus setting $\delta' = 0$ and substituting the result into (8.16b) yields

$$\begin{split} \delta'' &= f''(f - F) + f(f'' - F'') - 2(f')^2(f - F)/f \\ &\leq -2f(f - F) - 2(f')^2(f - F)/f \leq 0. \end{split}$$

We have shown that $\delta''(\theta) \le 0$ for any θ that satisfies $\delta'(\theta) = 0$; in view of Lemma 8.1, this yields a unique solution of (8.6) and hence results in a unique angle of propagation. \Box

For the simple case F = 0 or, more generally, F = constant, (8.12) yields

$$\mathbf{m}(\boldsymbol{\theta}) \cdot \mathbf{j} = \hat{\boldsymbol{\psi}}'(\boldsymbol{\theta}), \tag{8.17}$$

showing the extent to which anisotropy in the surface energy can negate the isotropic result $e(\theta) = j/|j|$.

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c. Comparison with the maximum energy release rate criterion

An alternative fracture criterion, due to COTTERELL (1965),¹⁹ asserts that the crack will propagate in a direction θ that maximizes the energy release rate $J(j,\theta)$. Since $J(j,\theta) = j \cdot e(\theta)$, this yields $e(\theta) = j/|j|$ and hence coincides with the prediction of the maximum dissipation criterion for a constitutively isotropic tip, but not generally for one that is anisotropic (*cf.* (8.12)). The possible extent of the difference is clear from the sentence containing (8.17).

If for an anisotropic tip the Cotterell criterion is interpreted to signify crack propagation in a direction that maximizes the *total* energy release rate $J(\mathbf{j}, \theta) - \hat{\psi}(\theta)$, then the predictions of the two criteria coincide provided both the limit force F and the mobility M are constant, but when this is not so the predictions of the two criteria still differ.

Of the two criteria, that of maximum dissipation seems more firmly rooted in thermodynamics: under isothermal conditions the maximum dissipation criterion is equivalent to the requirement that the crack propagate in a direction that maximizes the entropy production at the tip. Further, for a conservatively loaded elastic material, the maximum dissipation criterion ensures that the total energy decrease at a maximal rate.

¹⁹Cf. HUSSAIN, PU, and UNDERWOOD (1974), PALANISWAMY and KNAUSS (1978), COTTERELL and RICE (1980), LE (1989ab), STUMPF and LE (1990,1992).

9. CRYSTALLINE MATERIALS. A SKETCH

In this section we sketch a theory for the fracture of materials whose observed shapes are typically fully faceted. The surface energy of such a material, as a function of orientation, is nonsmooth with a nonconvex Frank diagram whose convexification is polygonal. The corresponding Wulff shape (the crystal shape that minimizes surface energy for a given volume of material) is then fully faceted, with facet-angles confined to the (finite) set Θ of angles that mark the vertices of the convexified Frank diagram. One method of analyzing such materials is to constrain the facet angles to the set Θ (cf., e.g., GURTIN (1993, § 12)). Likewise, we restrict to Θ the functions that specify a material's cracking response, and, for simplicity, assume that $F(\theta) \equiv 0$, so that the only impediment to fracture is the formation of new free surfaces. In addition, we restrict attention to materials with constant mobility. These constitutive assumptions, although oversimplified, hopefully convey the essence of the underlying physics.

Precisely, we assume that there is a finite orientation-set Θ consisting of angles θ at which the crack can propagate; angles other than those in Θ are not allowed. As before, we allow the energy to be a function

$$\psi_{\rm tip} = \hat{\psi}(\vartheta) \tag{9.1}$$

of the orientation of the free surface, but we consider $\hat{\psi}(\theta)$ as defined only when $\theta \in \Theta$. Let $\Omega(\hat{\psi})$ denote the finite set of points whose polar coordinates (r,θ) satisfy $r = \hat{\psi}(\theta)^{-1}$, $\theta \in \Theta$. We assume that there is a convex (closed) polygonal region, Polygon $(\hat{\psi})$, whose complete set of vertices coincides with $\Omega(\hat{\psi})$; the boundary of this polygon is what we shall consider as $Frank(\hat{\psi})$, the *Frank diagram* of $\hat{\psi}$, even though only its vertices correspond to possible angles of propagation.

Further, to simplify the discussion we limit our discussion to a linear relation between V and f with constant mobility M:

$$V(\Theta, f) = 0$$
 for $f \le 0$, (9.2a)

$$V(\theta, f) = Mf$$
 for $f > 0$, (9.2b)

with

$$M > 0. \tag{9.3}$$

We consider as criteria for initiation and fracture the conditions specified in

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Section 8, although the restriction to a constrained set of angles drastically changes the underlying picture, chiefly because $Frank(\hat{\psi})$, although convex, is not *strictly* convex.

The initiation condition (1.3) reduces to the Griffith condition

$$J(\mathbf{j}^+, \mathbf{\Theta}^+) = \hat{\Psi}(\mathbf{\Theta}^+), \tag{9.4}$$

and, since

$$\Gamma_{\rm tip}(j,\theta) = Mf^2, \quad f = f(j,\theta) = J(j,\theta) - \hat{\psi}(\theta),$$
(9.5)

the maximum dissipation criterion now has the form

$$\Gamma_{\rm tip}(\mathbf{j},\boldsymbol{\theta}) = \max_{\boldsymbol{\alpha} \in \mathcal{G}(\mathbf{j})} Mf^2(\mathbf{j},\boldsymbol{\alpha}), \tag{9.6a}$$

$$G(j) = \{ set of angles \ \theta \in \Theta \ such that \ J(j,\theta) > \hat{\psi}(\theta) \}.$$
 (9.6b)

Then, arguing as in Section 8, for a program of increasing loads $\operatorname{Frank}(J)$ will eventually touch $\operatorname{Polygon}(\hat{\psi})$ along $\operatorname{Frank}(\hat{\psi})$, and $\operatorname{fracture}$ will commence when a nontrivial interval of $\operatorname{Frank}(J)$ enters the interior of $\operatorname{Polygon}(\hat{\psi})$. At the instant before that happens the intersection of $\operatorname{Frank}(J)$ and $\operatorname{Frank}(\hat{\psi})$ will be either: (i) a single point, or (ii) a complete edge of $\operatorname{Frank}(\hat{\psi})$ In case (i) the intersection will take place at a vertex of $\operatorname{Frank}(\hat{\psi})$, the kink angle θ^+ will be the angle of that vertex, and the crack will run at the angle $\theta = \theta^+$ for a nontrivial interval of time. In case (ii) the intersection will include two vertices; if θ^+ and θ_+ are the corresponding angles, then either of these angles is a candidate for the kink angle, and perturbations in the loading or defects in the crystal would determine which of the two angles is chosen. Suppose now that the crack is propagating at a fixed angle $\theta = \theta^+$. The possibility then exists that the crack will kink again. Indeed, as the loading is increased the angle set G(j) may come to contain, in addition to θ^+ , a second angle θ_+ , and it is clear from (9.6a) that, depending on j, at some time it might happen that

$$f(j,\Theta_{+}) = f(j,\Theta^{+}).$$

At that time the minimal dissipation criterion does not yield a unique angle of propagation, and both θ^+ or θ_+ are candidates for the angle of propagation (Figure 6).



Figure 6

Frank diagrams of $\hat{\psi}$ and J for a crystalline material: (a) for a stationary crack; (b) for possible initiation of a running crack; (c) for a running crack; (d) for a possible kink from θ^* to θ_* (granted a = b).

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