



12-2011

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### Recommended Citation

Fu, Kai-Bin (2011). The Singular Perturbation in the Analysis of Mode I Fracture Based upon a New Multiscale Theory, *Applications and Applied Mathematics: An International Journal (AAM)*, Vol. 6, Iss. 2, Article 4.

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## The Singular Perturbation in the Analysis of Mode I Fracture Based upon a New Multiscale Theory

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Received: September 10, 2010; Accepted: September 3, 2011

### Abstract

A theory of fracture is presented that is based upon an extension of continuum mechanics to the nanoscale fracture through the incorporation of long-range intermolecular forces which correct bulk material descriptions near interfaces. To be consistent with the literature, constant surface energies are assigned to interfaces. In the analysis of mode I fracture for quasi-brittle material, it is observed that the incorporation of these long-range intermolecular forces predicts sharp fracture tip rather than blunt and avoids stress singularity. The details of the singular perturbation employed in this analysis are also presented.

**Keywords:** Fracture, intermolecular forces, singular perturbation, continuum mechanics

**MSC 2010:** 74A45; 35B25

### 1. Introduction

Understanding the fracture characteristics of semiconductor materials is crucial to modeling their mechanical response. The difficulties, both in experimental and theoretical fields, are obvious that the size of semiconductor materials is approaching nanoscale. There is a large and growing literature devoted to modeling and simulating fracture via atomistic simulation, molecular

dynamics or lattice dynamics methods [Fineberg et al. (1991), Marder & Gross (1995), Holland & Marder (1998), Slepyan et al. (1999), Abraham & Gao (2000), Abraham (2001), Swadener et al. (2002)]. Can continuum mechanics provide models capable of predicting or simulating nanoscale fracture problems? The work presented in this paper seeks to answer this question. Usually linear elastic fracture mechanics (LEFM) is assumed to be only applicable to linear elastic materials under quasistatic conditions. This classical theory, which originates from works of many authors [Griffith (1921), Williams (1957), Westergaard (1939), Irwin (1958)], predicts an infinite stress at the crack tip.

Barenblatt (1962) and Dugdale (1960) introduced the so-called cohesive zone model. Compressional cohesive stresses are distributed over a small region near the crack tip. The cohesive zone has its own constitutive equations which is often determined arbitrarily. Gurtin (1979a) introduced thermodynamics into the cohesive zone models. Since then, cohesive zone models have been developed and applied to a variety of fracture problems [Schapery (1975), Knauss (1993), Costanzo & Allen (1995), Hui et al. (1987), Costanzo & Walton (1997)]. Eringen (1972a) developed the nonlocal continuum theory and applied it to some crack problems [Eringen et al. (1977), Eringen (1981), Ari & Eringen (1983)]. In the approach of nonlocal continuum theory, the stress at a point is influenced by the strain field at all points of the body. By using proper nonlocal kernel and boundary conditions, stress singularities at the crack tip are eliminated. Other non-elastic models such as plastic zone [Irwin (1961)] have also been proposed to reduce stress singularities in last several decades.

This continuum approach to nanoscale fracture modelling is based upon a new theory of extension of continuum mechanics to the nanoscale [Slattery et al. (2004)]. In the immediate neighborhood of a phase interface, material behavior differs from that observed at some distance from the interface. All (local) descriptions of material behavior at some distance from the interface are based upon the assumption that the material extends to "infinity" (perhaps 100 nm) in all directions. Material points outside the immediate neighborhood of the interface are subjected to intermolecular forces only from one phase. Material points within the immediate neighborhood of a phase interface are subjected to intermolecular forces from both phases. Intermolecular forces are taken into account with an appropriate bulk description for material behavior. An unusual aspect of this approach is that it proves more convenient to linearize the equations of elasticity about the deformed configuration in which the crack is open. This is in contrast to classical linear elastic fracture mechanics in which the linearization is relative to a reference configuration with the crack modeled as a virtual, unopened slit. In particular, it is more convenient to discuss the correction to bulk stress-deformation in the deformed frame than in the undeformed frame.

The continuum approach based on bulk descriptions of behavior, for example, bulk stress-deformation behavior, has been applied to fracture problems. The bulk descriptions of behavior assume that the material extends to "infinity" (perhaps 100 nm) in all directions. This approach showed that, in the limit as the crack tip was approached, stresses became proportional to  $r^{-1/2}$  regardless of geometry and applied loading, in which  $r$  was the radial distance measured from the crack tip [Westergaard (1934), Westergaard (1939), Williams (1957, 1959)].

That the stress becomes unbounded as the crack tip is approached suggests that this approach fails to describe the physics correctly in the neighborhood of the crack tip. In fact, within the immediate neighborhood of crack surfaces including the crack tip, the material is subjected to long-range intermolecular forces from the adjoining phase, and the observed material behavior is different from the bulk material behavior.

An obvious approach to nanoscale modeling of fracture is to employ molecular dynamics or lattice fracture methodologies [Fineberg et al. (1991), Marder & Gross (1995), Holland & Marder (1998), Slepyan et al. (1999), Abraham & Gao (2000), Abraham (2001), Swadener et al. (2002)]. A major difficulty that one immediately encounters in attempting to attack such problems using a molecular description of the material is the specification of the intermolecular forces [Holland & Marder (1998)]. This can be done exceptionally well for dilute gases, but is more problematic for liquids and solids. Alternatively, attempting to apply non-local continuum theories of material behavior in these interfacial regions is hampered by the difficulty of measuring local stress-deformation behavior at such small scales.

Proposed herein is a novel extension of continuum mechanics to the near molecular scale to treat nanoscale fracturing. For the interfacial region such as the immediate neighborhood of the crack surface, this theory employs known bulk material behavior corrected for the intermolecular forces from the adjoining phase. As such, the theory is expected to be much less sensitive to the choice of intermolecular force potential upon knowing bulk material properties (suitably far away from phase interfaces) and merely uses the intermolecular force potential to construct a correction to bulk properties in the vicinity of phase interfaces. Evidence that this expectation is valid has been provided by the recent successful application of this theory in the context of supercritical adsorption, contact angles, surface energy [Fu et al. (2004), Slattery et al. (2004)].

Linear elastic fracture (LEFM) mechanics is arguably one of the most successful theories in all of applied continuum mechanics. Its literature is vast and it has been applied to countless practical fracture problems for brittle solids exhibiting small, very limited amounts of inelastic or dissipative fracture processes. However, this record of successful applications has been achieved in spite of the theory's nagging logical inconsistencies and physically impossible predictions. For example, while the theory is set within the context of the linearized equations of elasticity, which is predicated upon the assumption of infinitesimally strains, it predicts strains and stresses of unbounded size in the immediate neighborhood of a crack edge. Even worse, when applied to fractures occurring along an interface between two distinct solid phases, it predicts interpenetration of the two fracture surfaces.

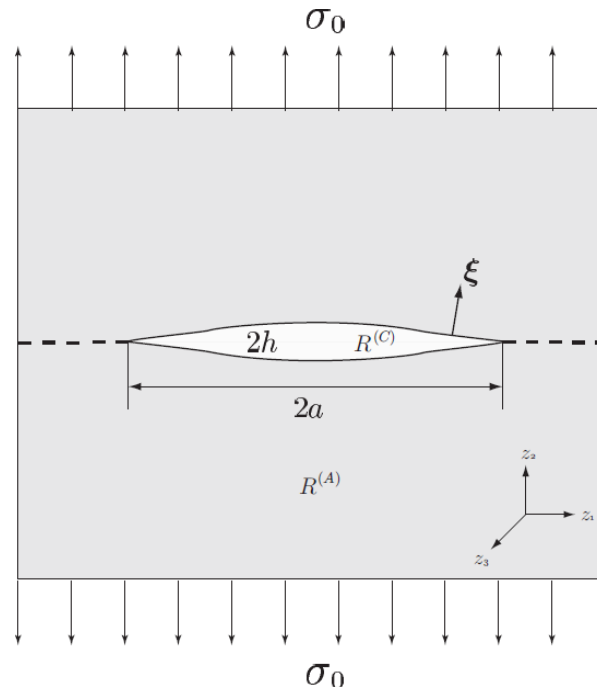
There have been many strategies proposed for rationalizing, resolving or avoiding these logical inconsistencies. Early on in the development of the theory when these inconsistencies were first encountered, some argued that they could be ignored without harm to the successful application of the theory to practical problems. The rationale for this view was that physically unrealistic magnitudes for stresses and strains predicted by the theory occur only in a region very near to a fracture edge and that, since the theory predicts finite fracture energies, a rational fracture criterion based upon the fracture energy release rate could be implemented in spite of the infinitely large stresses and strains and material interpenetration, at least in the context of quasi-static or equilibrium fracture problems. Others argued that the inconsistencies could be avoided

by setting elastic fracture mechanics within the context of finite elasticity. However, when the classical boundary conditions used to model a fracture front are imposed upon the equations of finite elasticity, theory still predicts infinite stresses. Still others have contended that the inconsistencies are due to the nature of the boundary conditions arising from the classical idealized view of a fracture edge. More specifically, a fracture has been classically modeled as a surface (in the material body's reference configuration, say) across which the displacement vector has a discontinuity. The boundary of this fracture surface is a curve representing an idealized fracture edge or front. The boundary conditions specify the traction on the fracture surface, resulting in a sudden change in the boundary conditions across the fracture edge. It was then argued by many researchers that one should give a fracture edge or zone a two (cohesive zone) or three (process zone) dimensional structure, in order to prevent the development of unbounded stresses and strains. Many such analyses have appeared in the literature in the context of both linear and finite elasticity. Despite its obvious virtues, this approach is not without its own thorny difficulties, both theoretical and practical. For one thing, many implementations of either cohesive or process zone models employ constitutive relations for the cohesive or process zone of dubious physical basis. Moreover, determining constitutive response functions for either a cohesive or process zone model from experimental observation is highly problematical.

Some have argued that, since in real materials fracture occurs via nano or molecular scale processes, one should not hope to be able to model it consistently or effectively within the context of continuum mechanics. Consequently, there is also a large and growing literature devoted to modeling and simulating fracture via molecular dynamics or lattice fracture methodologies [Fineberg et al. (1991), Marder & Gross (1995), Holland & Marder (1998), Slepyan et al. (1999), Abraham & Gao (2000), Abraham (2001), Swadener et al. (2002)]. A major difficulty that one immediately encounters in attempting to attack such problems using a molecular description of the material is the specification of the intermolecular forces (Holland & Marder 1998). This can be done exceptionally well for dilute gases, but is more problematic for liquids and solids. Alternatively, attempting to apply non-local continuum theories of material behavior in these interfacial regions is hampered by the difficulty of measuring local stress-deformation behavior at such small scales.

The continuum approach to fracture modelling is based on bulk descriptions of behavior, for example, bulk stress-deformation behavior. This bulk description of stress deformation behavior assumes that, about each material point, the material extends to "infinity" (perhaps 100 nm) in all directions. However, within the immediate neighborhood of crack surfaces, including the crack tip, the material is subjected to long-range intermolecular forces from the adjoining phases, and the observed material behavior is different from the bulk material behavior.

An unusual aspect of this approach is that it proves more convenient to linearize the equations of elasticity about the deformed configuration in which the crack is open. This is in contrast to classical linear elastic fracture mechanics in which the linearization is relative to a reference configuration with the crack modeled as a virtual, unopened slit. In particular, it is more convenient to discuss the correction to bulk stress-deformation in the deformed frame than in the undeformed frame.



**Figure 1.** Schematic of Mode I fracture of phase *C* in phase *A*.

Oh et al. (2006) have reviewed the development of the fracture mechanics literature, and we will not repeat it here.

Slattery et al. (2004) have presented a theory extending continuum mechanics to the immediate, nanoscale neighborhood of a phase interface, where the behavior of a phase is altered by the intermolecular forces from the adjoining phase. It employs known bulk material behavior with a mutual body force correction for the intermolecular forces from adjoining phases. Expanding upon Slattery et al. (2004), Oh et al. (2006) have described six views of the interfacial region, and they have employed view (iv) in analyzing a static mode I fracture. In view (iv), the surface energy  $\gamma$  varies as a function of position in the immediate neighborhood of the fracture tip.

Here we adopt view (v) of Oh et al. (2006) to solve the same problem. In view (v), we use the more common assumption that surface energy is independent of position, with the value that would be appropriate, if both phases adjoining the interface were semi-infinite, rather than one being a thin gas film.

## 2. Problem statement

Figure 1 shows a static Mode I fracture with an applied stress  $\sigma_0$  for quasi-brittle material. The length of the fracture is specified to be  $a$ .  $2h$  is the distance between upper surface and lower surface of the crack, which is better understood with 2. Our objective is to solve the differential momentum balance (1) consistent with the jump momentum balance (2) and to determine both

the crack configuration and the stress distribution in the solid, particularly within the immediate neighborhood of the fracture tip.

In the immediate neighborhood of a phase interface, material behavior differs from that observed at some distance from the interface. All (local) descriptions of material behavior at some distance from the interface are based upon the assumption that the material extends to "infinity" (perhaps 100 nm) in all directions. Material points outside the immediate neighborhood of the interface are subjected to intermolecular forces only from one phase. Material points within the immediate neighborhood of a phase interface are subjected to intermolecular forces from both phases. Our premise is that material behavior within the interfacial region can be represented as bulk material behavior corrected for the intermolecular forces from the adjoining phase. In particular, we recognize the equivalence of stresses and body forces [Truesdell & Toupin (1960, p. 549)].

We make several assumptions.

- 1) We have followed those descriptions of a material interface in Slattery et al. (2004) and Oh et al. (2006). While we will not repeat those descriptions, here we show more details of view (d) in Slattery et al. (2004) and view (v) in Oh et al. (2006) which is used in this analysis.

We recommend as an approximation that dividing surfaces be introduced with constant values of surface tension or energy  $\gamma^\infty$  that correspond to static, unbounded dividing surfaces. These would be the surface tensions or energies commonly used. The correction potential  $\Phi^{(A, corr)^\infty}$  must of course be modified to account for these surface tensions or energies. With this point of view, the differential momentum balance becomes

$$\text{div } \mathbf{T}^{(\mathbf{l}, \text{bulk})^\infty} - \nabla \Phi^{(A, \text{corr})^\infty} = \mathbf{0} \quad (1)$$

and jump momentum balance becomes

$$2H \gamma^\infty \boldsymbol{\xi} + [\mathbf{T}^{(\mathbf{l}, \text{bulk})^\infty} \boldsymbol{\xi}] = \mathbf{0} \quad (2)$$

Here  $H$  is the mean curvature,  $\boldsymbol{\xi}$  is the unit normal to the crack surface point into the solid.

- 2) We assume that the point-to-point intermolecular force potential can be represented as

3)

$$\phi^{(A,C)} = -\frac{A^{(A,C)}}{\pi^2 n^{(A)^2} r^6} \quad (3)$$

where  $A^{(A,C)}$  is the effective, Lifshitz type, Hamaker constant between phases  $A$  and  $C$  [Bowen & Jenner (1995), Lifshitz (1956)]. The Hamaker constants of most condensed phases are found to lie in the range of  $0.4-4 \times 10^{-20}$  J [Israelachvili (1991, p.176)].

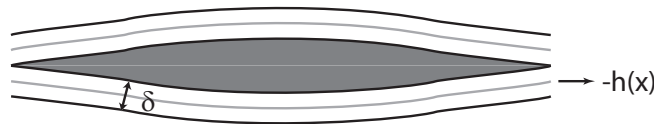
The analysis is in the context of linear elasticity with assumption 1. Each crack face is regarded as a single dividing surface with a constant surface energy  $\gamma^\infty$ . As described in 2, Sec. 4.1 [Slattery et al. (2004)],  $\gamma^\infty$  cannot fully account for the correction that must be made to the intermolecular forces. An additional correction  $\Phi^{(A,corr)\infty}$  should be made. Two crack surfaces could be viewed as discontinuous thin films. Because a constant surface energy stands for the work to separate two materials from contact to infinity, we treat crack surfaces as infinite continuous thin films in the computation of  $\Phi^{(A,corr)\infty}$ .

$$\begin{aligned} \Phi^{(A,corr)\infty} &= -\int_{R^{(A)}} [n^{(A)}n^{(C)}\phi^{(A,C)} - n^{(A)}n^{(A)}\phi^{(A,A)} - n^{(C)}n^{(C)}\phi^{(C,C)} + n^{(A)}n^{(C)}\phi^{(A,C)}] dr \\ &\cong -\frac{A}{\pi^2} \int_{-a}^a \int_{-\infty}^{-h(x)-\delta/2} \int_{-\infty}^{\infty} \frac{1}{[(z_1-x)^2 + (z_2-y)^2 + z^2]^3} dz dy dx \end{aligned} \quad (4)$$

The first equation is derived from Eq. 41 [Slattery et al. (2004)]. The second approximation is concluded from the asymptotic expansions executed later. Here we only write the significant contribution of  $\Phi^{(A,corr)\infty}$  to simplify the expression. For the same reason, we define

$$A \equiv -(2A^{(AC)} - A^{(AA)} - A^{(CC)}) \quad (5)$$

$\delta$  in Figure 2 is the distance separating the two phases  $A$  and  $C$ , corresponding physically to the sum of the effective radii of the  $A$  and  $C$  molecules or the effective distance between molecules of  $A$  and  $C$  [Slattery et al. (2004, p.4623)]. The dividing surface  $h(x)$  is located halfway between the two phases.



**Figure 2.**  $\delta$  is the distance separating the two phases  $A$  and  $C$ , corresponding physically to the sum of the effective radii of the  $A$  and  $C$  molecules or the effective distance between molecules of  $A$  and  $C$  [Slattery et al. 2004]. The dividing surface  $h(x)$  is located halfway between the two phases.

4) It is assumed that  $T^{(l, bulk)\infty}$  can be described by Hooke's law

$$\mathbf{T}^{(l, bulk)\infty} = \frac{\gamma E}{(1+\gamma)(1-2\gamma)} (tr \mathbf{e}) \mathbf{I} + \frac{E}{(1+\gamma)} \mathbf{e} \quad (6)$$

in which

$$\mathbf{e} \equiv \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad (7)$$



is the infinitesimal strain tensor.

5) Gravitational and inertial effects are neglected.

### 3. Solution

Let's introduce dimensionless variables:

$$\begin{aligned} \mathbf{u}^* &\equiv \mathbf{u}/a, & z_i^* &\equiv z_i/a, & \mathbf{h}^* &\equiv \mathbf{h}/a, & \delta^* &\equiv \delta/a \\ A^* &\equiv A/(\pi^2 E a^3), & H^* &\equiv H a, & \gamma^* &\equiv \gamma^\infty / E a \end{aligned} \quad (8)$$

In terms of these dimensionless variables, the differential momentum balance (1) can be expressed as

$$\frac{\gamma^*}{(1+\gamma^*)(1-2\gamma^*)} \Delta \mathbf{u}^* + \frac{1}{2(1+\gamma^*)(1-2\gamma^*)} \nabla \operatorname{div} \mathbf{u}^* - \nabla \Phi^* = 0 \quad (9)$$

and the jump momentum balance (2) can be rewritten as

$$2H^* \gamma^* \boldsymbol{\xi} + \frac{\gamma^*}{(1+\gamma^*)(1-2\gamma^*)} (\nabla \mathbf{u}^* + \nabla \mathbf{u}^{*\top}) \boldsymbol{\xi} + \frac{1}{2(1+\gamma^*)} (\operatorname{div} \mathbf{u}^*) \boldsymbol{\xi} = \mathbf{0}, \quad (10)$$

where

$$\Phi^*(z_1^*, z_2^*) = A^* \int_{-1}^1 \int_{-\infty}^{-h^*(x) - \delta^*/2} \int_{-\infty}^{\infty} \frac{1}{[(z_1^* - x^*)^2 + (z_2^* - y^*)^2 z^{*2}]^3} dz^* dy^* dx^*. \quad (11)$$

This expression depends upon the crack face profile  $h(x)$  which is unknown a priori and must be determined as part of the problem's solution. However, two of the three iterated integrals can be evaluated in closed form using elementary techniques. In particular, one readily shows that

$$\begin{aligned} &\Phi^*(z_1^*, z_2^*) \\ &= \frac{A^* \pi}{4} \int_{-1}^1 \left\{ 1 - \frac{(2(h^*(x^*) + \delta^*/2) + 2z_2^*) [6(z_1^* - x^*)^2 + (2(h^*(x^*) + \delta^*/2) + 2z_2^*)^2]}{[4(z_1^* - x^*)^2 + (2(h^*(x^*) + \delta^*/2) + 2z_2^*)^2]^{3/2}} \right\} \frac{dx^*}{(z_1^* - x^*)^4} \end{aligned} \quad (12)$$

We approximate the integral expression (12) with the assumption that  $h(x)$  is locally constant. Mathematically it requires that  $h(x)$  is slowly varying such that the magnitude of its derivative  $|h'(x)|$  is small. Physically it means that we compute  $\Phi^*$  for any point at the crack surfaces as a

point at the parallel plane interfaces [Sec. 4.1.1](Slattery et al. 2004). This assumption will then be verified à posteriori for consistency. Therefore, we have the analytical expression for  $\Phi^*$

$$\Phi^*(z_1^*, z_2^*) = A^* \left\{ \begin{aligned} & \frac{1}{12(z_1^* - 1)^3} - \frac{1}{12(z_1^* + 1)^3} + \frac{2(z_1^* + 1)^4 + (z_1^* + 1)^2(z_2^* + h^* + \delta^*/2)^2 + 2(z_2^* + h^* + \delta^*/2)^4}{24(z_1^* + 1)^3(z_2^* + h^* + \delta^*/2)^3 \sqrt{(z_1^* + 1)^2 + (z_2^* + h^* + \delta^*/2)^2}} \\ & - \frac{2(z_1^* - 1)^4 + (z_1^* - 1)^2(z_2^* + h^* + \delta^*/2)^2 + 2(z_2^* + h^* + \delta^*/2)^4}{24(z_1^* - 1)^3(z_2^* + h^* + \delta^*/2)^3 \sqrt{(z_1^* - 1)^2 + (z_2^* + h^* + \delta^*/2)^2}} \end{aligned} \right\} \quad (13)$$

### A. Singular perturbation method

We seek a solution with the perturbation method. As stated in assumption 2, the Hamaker constant is very small. We choose the dimensionless Hamaker constant  $A^*$  as the perturbation parameter. When  $A^* = 0$ , our theory demands that there must be no fracture. However, as  $A^* \rightarrow 0$ , the solution does not approach this limit. For this reason, the perturbation analysis performed for this problem is singular Bush (1992, p.11).

Due to the singular nature of the problem, a single asymptotic expansion cannot be valid in the entire body. Thus, we develop two solutions: the *outer solution*, which represents the smoothly changing portion, and the *inner solution*, which represents the rapidly changing portion in the immediate neighborhood of crack surfaces. For the boundary conditions, we need to apply the method of matched asymptotic expansions [Kevorkian & Cole (1981)]. We force outer solution and inner solution to be identical at some point. In this analysis, it is when  $y_2^{**} \rightarrow \infty$ .

1) *Outer solution*: The outer solution corresponds to  $A^* = 0$ , a uniaxial extension upon a body without a crack.

$$T_{22}^{(I,bulk)\infty*} = \sigma_0^* \quad (14)$$

$$u_1^* = -\gamma(1 + \gamma)\sigma_0^* z_1^* \quad (15)$$

$$u_2^* = (1 - \gamma)^2 \sigma_0^* z_2^* \quad (16)$$

where

$$T_{22}^{(I,bulk)\infty*} \equiv \frac{T_{22}^{(I,bulk)\infty}}{E}, \quad \sigma_0^* \equiv \frac{\sigma_0}{E} \quad (17)$$

2) *Inner solution*: Within the immediate neighborhood of the crack surfaces (inner region),  $\Phi^*$  must be preserved. This suggests that we introduce as expanded variables in this region

$$y_2^{**} \equiv \frac{z_2^* - h^*}{A^{*n}} \quad (18)$$

$$v_2^{**} \equiv \frac{u_2^* - h^*}{A^{*n}} \quad (19)$$

$$\delta^{**} \equiv \frac{\delta^*}{2A^{*n}} \quad (20)$$

The exponent  $n$  is chosen in (21) so that the effect of the long-range intermolecular forces is retained as  $A^* \rightarrow 0$ . Note that, with this value of  $n$ ,

$$\delta^{**} = \frac{\delta\pi^{2/3}E^{1/3}}{2A^{1/3}} = \text{constant} \quad (21)$$

In terms of these scaled variables, the two components of the differential momentum balance (9) become

$$\begin{aligned} & \left\{ (\lambda^* + 2\mu^*) \frac{\partial^2 u_1^*}{\partial z_1^{*2}} + (\lambda^* + \mu^*) \frac{\partial^2 v_2^{**}}{\partial z_1^* \partial y_2^{**}} \right\} + \frac{1}{A^{*2n}} \left\{ (\lambda^* + 2\mu^*) \left( \frac{dh^*}{dz_1^*} \right)^2 + \mu^* \frac{\partial^2 u_1^*}{\partial y_2^{**2}} \right\} \\ & - \frac{1}{A^{*n}} \left\{ (\lambda^* + 2\mu^*) \frac{dh^*}{dz_1^*} \frac{\partial^2 u_1^*}{\partial z_1^* \partial y_2^{**}} - (\lambda^* + 2\mu^*) \frac{d^2 h^*}{dz_1^{*2}} \frac{\partial u_1^*}{\partial y_2^{**}} - (\lambda^* + \mu^*) \frac{dh^*}{dz_1^*} \frac{\partial^2 v_2^{**}}{\partial y_2^{**2}} \right\} = \frac{\partial \Phi^{**}}{\partial z_1^*} \end{aligned} \quad (22)$$

and

$$\begin{aligned} & A^{*n} \mu^* \frac{\partial^2 v_2^{**}}{\partial z_1^{*2}} + \left\{ \mu^* \frac{d^2 h^*}{dz_1^{*2}} - \mu^* \frac{d^2 h^*}{dz_1^{*2}} \frac{\partial v_2^{**}}{\partial y_2^{**}} - 2\mu^* \frac{dh^*}{dz_1^*} \frac{\partial^2 v_2^{**}}{\partial z_1^* \partial y_2^{**}} \right\} - \frac{1}{A^{*2n}} \left\{ (\lambda^* + \mu^*) \frac{dh^*}{dz_1^*} \frac{\partial^2 u_1^*}{\partial y_2^{**2}} \right\} \\ & \frac{1}{A^{*n}} \left\{ (\lambda^* + 2\mu^*) \frac{\partial^2 v_2^{**}}{\partial y_2^{**2}} + \mu^* \frac{dh^*}{dz_1^*} \frac{\partial^2 v_2^{**}}{\partial z_1^* \partial y_2^{**2}} + (\lambda^* + \mu^*) \frac{\partial^2 u_1^*}{\partial z_1^* \partial y_2^{**}} \right\} = \frac{\partial \Phi^{**}}{\partial y_2^{**}} \end{aligned} \quad (23)$$

We have assumed that  $h^*$  is slowly varying, permitting us to neglect both the first and second derivatives of  $h^*$  over  $z_1^*$ . We can work on the simplified form of (22) and (23)

$$A^{*-2n} \mu^* \frac{\partial^2 u_1^*}{\partial y_2^{**2}} + (\lambda^* + 2\mu^*) \frac{\partial^2 u_1^*}{\partial z_1^{*2}} + (\lambda^* + \mu^*) \frac{\partial^2 v_2^{**}}{\partial z_1^* \partial y_2^{**}} = \frac{\partial \Phi^{**}}{\partial z_1^*} \quad (24)$$

and

$$A^{*2n} \mu^* \frac{\partial^2 v_2^{**}}{\partial z_1^{*2}} + A^{*n} \mu^* \frac{\partial^2 h^*}{\partial z_1^{*2}} + (\lambda^* + 2\mu^*) \frac{\partial^2 v_2^{**}}{\partial y_2^{**2}} + (\lambda^* + \mu^*) \frac{\partial^2 u_1^*}{\partial z_1^* \partial y_2^{**}} = \frac{\partial \Phi^{**}}{\partial y_2^{**}} \quad (25)$$

Here

$$\begin{aligned} & \Phi^{**}(z_1^*, y_2^{**}) \\ &= A^{*1-3n} \left\{ \begin{aligned} & \frac{(A^*)^{3n}}{12(z_1^* - 1)^3} - \frac{(A^*)^{3n}}{12(z_1^* + 1)^3} \\ & + \frac{2(z_1^* + 1)^4 + (A^*)^{2n}(z_1^* + 1)^2(y_2^{**} + 2h^{**} + \delta^{**})^2 + 2(A^*)^{4n}(y_2^{**} + 2h^{**} + \delta^{**})^4}{24(z_1^* + 1)^3(y_2^{**} + 2h^{**} + \delta^{**})^3 \sqrt{(z_1^* + 1)^2 + (A^*)^{2n}(y_2^{**} + 2h^{**} + \delta^{**})^2}} \\ & - \frac{2(z_1^* - 1)^4 + (A^*)^{2n}(z_1^* - 1)^2(y_2^{**} + 2h^{**} + \delta^{**})^2 + 2(A^*)^{4n}(y_2^{**} + 2h^{**} + \delta^{**})^4}{24(z_1^* - 1)^3(y_2^{**} + 2h^{**} + \delta^{**})^3 \sqrt{(z_1^* - 1)^2 + (A^*)^{2n}(y_2^{**} + 2h^{**} + \delta^{**})^2}} \end{aligned} \right\} \quad (26) \end{aligned}$$

If the contribution of  $\Phi^{**}$  in (24) and (25) is to be the same order of magnitude as the other terms when  $A^* \rightarrow 0$ , we must identity

$$n = \frac{1}{3} \quad (27)$$

In view of (27), equations (24) and (25) reduce to

$$\frac{\partial^2 u_1^*}{\partial y_2^{**2}} = 0 \quad (28)$$

$$(\lambda^* + 2\mu^*) \frac{\partial^2 v_2^{**}}{\partial y_2^{**2}} + (\lambda^* + \mu^*) \frac{\partial^2 u_1^{**}}{\partial z_1^* \partial y_2^{**}} = \frac{\partial \Phi^{**}}{\partial y_2^{**}} \quad (29)$$

Equations (28) and (29) are satisfied with

$$u_1^* = a(z_1^*)y_2^{**} + b(z_1^*) \quad (30)$$

and

$$(\lambda^* + 2\mu^*) v_2^{**} = \int \Phi^{**} dy_2^{**} + f(z_1^*)y_2^{**} - \frac{\lambda^* + \mu^*}{2} \frac{\partial a(z_1^*)}{\partial z_1^*} y_2^{**2} + g(z_1^*) \quad (31)$$

Functions  $a(z_1^*)$ ,  $b(z_1^*)$ ,  $f(z_1^*)$  and  $g(z_1^*)$  can be obtained using the boundary conditions. On the crack surfaces, the two components of (10) are expressed in terms of  $y_2^*$  and  $v_2^*$

$$\frac{\partial^2 h^*}{\partial z_1^{*2}} \left\{ 1 + \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 \right\}^{\frac{3}{2}} \gamma^* \left( \frac{\partial h^*}{\partial z_1^*} \right) + \left[ (\lambda^* + 2\mu^*) \frac{\partial u_1^*}{\partial z_1^*} + \lambda^* \frac{\partial v_2^*}{\partial y_2^*} \right] \left( -\frac{\partial h^*}{\partial z_1^*} \right) + \mu^* \left[ \frac{\partial v_2^*}{\partial z_1^*} + \frac{\partial h^*}{\partial z_1^*} + \frac{\partial u_1^*}{\partial y_2^*} \right] = 0 \quad (32)$$

and

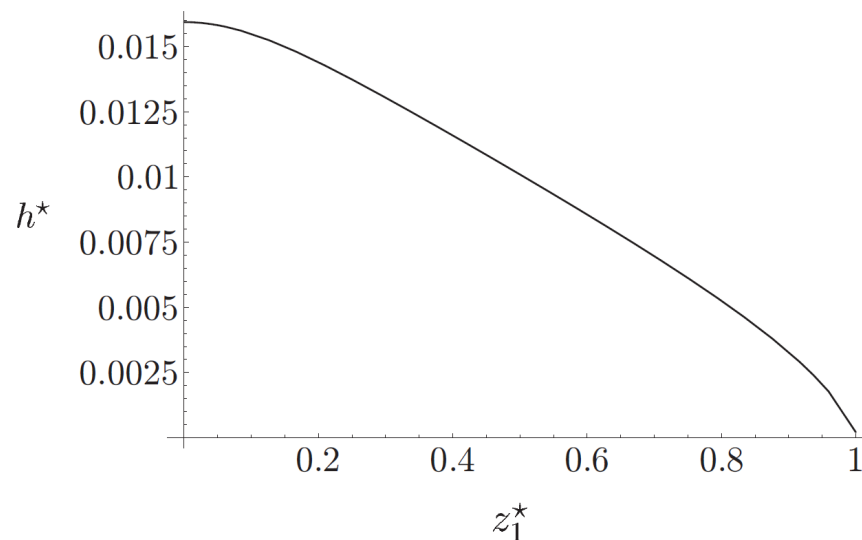
$$\frac{\partial^2 h^*}{\partial z_1^{*2}} \left\{ 1 + \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 \right\}^{\frac{3}{2}} \gamma^* + \mu^* \left[ \frac{\partial v_2^*}{\partial z_1^*} + \frac{\partial h^*}{\partial z_1^*} + \frac{\partial u_1^*}{\partial y_2^*} \right] \left( -\frac{\partial h^*}{\partial z_1^*} \right) + \left[ (\lambda^* + 2\mu^*) \frac{\partial v_2^*}{\partial y_2^*} + \lambda^* \frac{\partial u_1^*}{\partial z_1^*} \right] = 0 \quad (33)$$

In terms of  $y_2^{**}$  and  $v_2^{**}$ , these become

$$\frac{\partial u_1^*}{\partial y_2^{**}} = 0 \quad (34)$$

and

$$\frac{\partial^2 h^*}{\partial z_1^{*2}} \gamma^* + \left\{ 1 + \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 \right\}^{\frac{3}{2}} \left\{ -\mu^* \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 + \left[ (\lambda^* + 2\mu^*) \frac{\partial v_2^{**}}{\partial y_2^{**}} + \lambda^* \frac{\partial u_1^*}{\partial z_1^*} \right] \right\} = 0 \quad (35)$$



**Figure 3.** Dimensionless crack configurations  $h^*$  for  $\delta^* = 0.02$  and  $\delta^{**} = 2.50$ . Here we have used  $E = 100$  GPa,  $\delta = 0.2$  nm,  $a = 10$  nm, and  $A = 2\pi \times 10^{-20}$  J.

One of these components of the jump momentum balance allows us to obtain a configuration of the dividing surface.

As  $y_2^{**}$  approaches infinity, the body force correction term will disappear and we also require that the inner solutions given as (30) and (31) should approach asymptotically the corresponding solutions in the outer region:

as

$$y_2^{**} \rightarrow \infty : \quad u_1^* \rightarrow -\frac{\lambda^*}{4\mu^*(\lambda^* + \mu^*)} \sigma_0^* z_1^* \quad (36)$$

$$T_{22}^* \rightarrow \sigma_0^* \quad (37)$$

$$\Phi^{**} \rightarrow 0 \quad (38)$$

In view of (34), (36), (37) and (38), we have

$$a(z_1^*) = 0 \quad (39)$$

$$b(z_1^*) = -\frac{\lambda^*}{4\mu^*(\lambda^* + \mu^*)} \sigma_0^* z_1^* \quad (40)$$

$$f(z_1^*) = \sigma_0^* \left[ 1 + \frac{\lambda^{*2}}{4\mu^*(\lambda^* + \mu^*)} \right] \quad (41)$$

so that the inner solutions given as (30) and (31) become

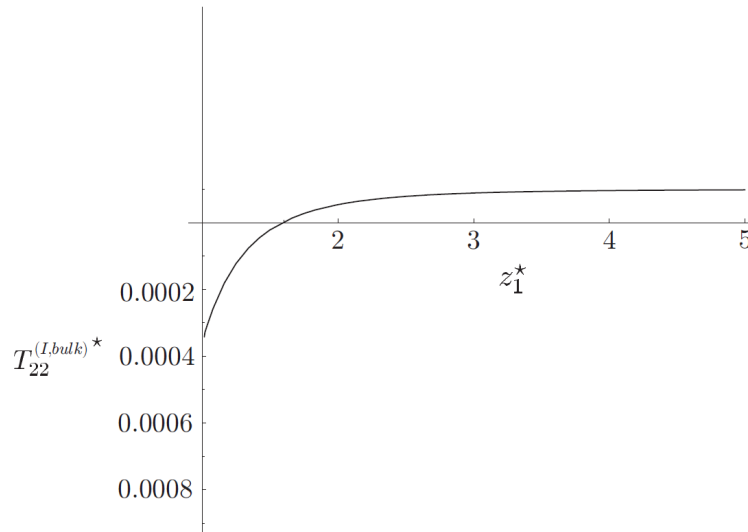
$$u_1^* = -\frac{\lambda^*}{4\mu^*(\lambda^* + \mu^*)} \sigma_0^* z_1^* \quad (42)$$

and

$$(\lambda^* + 2\mu^*) v_2^{**} = \int \Phi^{**} dy_2^{**} + \sigma_0^* \left[ 1 + \frac{\lambda^{*2}}{4\mu^*(\lambda^* + \mu^*)} \right] y_2^{**} + g(z_1^*) \quad (43)$$

Using (42) and (43), we express the stress in inner region as

$$T_{22}^{(I, bulk) \infty} \equiv (\lambda^* + 2\mu^*) \frac{\partial v_2^{**}}{\partial y_2^{**}} + \lambda^* \frac{\partial u_1^*}{\partial z_1^*} = \Phi^{**} + \sigma_0^* \quad (44)$$



**Figure 4.** Dimensionless stress distribution  $T_{22}^{(I,bulk)*}$  on the fracture axis for  $\delta^* = 0.02$  and  $\delta^{**} = 2.50$ . Here we have used  $E = 100$  GPa,  $\delta = 0.2$  nm,  $a = 10$  nm, and  $A = 2\pi \times 10^{-20}$  J.

Substituting (42) and (43) into (35), we will have

$$\frac{\partial^2 h^*}{\partial z_1^{*2}} \gamma^* + \left\{ 1 + \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 \right\}^{\frac{3}{2}} \left\{ \sigma_0^* - \mu^* \left( \frac{\partial h^*}{\partial z_1^*} \right)^2 + \Phi^{**} \right\} = 0 \quad (45)$$

We can obtain configurations of crack surfaces from Equation (45). Since this is a second-order differential equation, we need two boundary conditions as follows:

$$\text{at } z_1^* = 0: \quad \frac{\partial h^*}{\partial z_1^*} = 0 \quad (46)$$

$$\text{at } z_1^* = 1: \quad h^* = \frac{\delta^*}{2} \quad (47)$$

The first reflects symmetry with respect to the crack surface. At the crack tip, there is only a separation distance between two crack surfaces. This problem was solved using the Mathematica Software package.

#### 4. Discussion

The first reflects symmetry with respect to the crack surface. At the crack tip, there is only a separation distance between two crack surfaces. This problem was solved using the Mathematica software package.

The results developed here are similar to those presented by Oh et al. 2006 with one important exception. Oh et al. 2006 show that the stress in the immediate neighborhood of the fracture tip is tensile, which is physically appealing like most classical theories do. Figure 4 indicates that it is compressive. Unfortunately, to our knowledge there are no experimental data available with which to compare the two results. We believe, however that this analysis is physically sound and will have experimental support eventually.

Oh et al. 2006 takes the view that all of the correction of the intermolecular forces account into the variable surface energy. This analysis takes the view that the correction of the intermolecular forces is composed of two parts: a constant surface energy, which is more common in the literature, and an additional correction term contributed from intermolecular forces. It is interesting that, when we think about computing the energy release rate following the definition of Gurtin 1979(b), the view of a constant surface energy taken in this paper appears to be more appropriate.

One thing we want to point out is that the use of singular perturbation in this analysis is unique. It is our novel idea to draw the analogy between boundary layer theory for fluid flow and the immediate neighborhood of crack surfaces.

This analysis only deals with one pre-existing crack. The analysis of multiple cracks is saved for future study and will be included in another manuscript.

### ***Acknowledgement***

*The author acknowledges the support provided by the National Science Foundation under grant CMS-030927 and Air Force Office of Scientific Research under grant FA9550-06-1-0242. We are also grateful for the many extended conversations with Dr. John C. Slattery and Dr. Eun-Suok Oh.*

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