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A FRAMEWORK TO CORRELATE EFFECTS OF CONSTRAINT LOSS AND DUCTILE TEARING ON FRACTURE TOUGHNESS – PART I : PROBABILISTIC APPROACH

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Abstract *– This study explores the development of a probabilistic (micromechanics) framework applicable to cleavage fracture to predict effects of constraint loss and ductile tearing on macroscopic fracture toughness (J_c). Specifically, a probabilistic model employing the statistics of microcracks (weakest link philosophy) and a local failure criterion for transgranular cleavage provides the coupling between the microregime of fracture (which includes the stresses that develop ahead of the macroscopic crack) with macroscopic (remote) loading. For stress-controlled, cleavage mechanisms of material failure, the Weibull stress (σ_w) emerges as a probabilistic fracture parameter defining conditions leading to (local) fracture. This parameter permits predictions of the strong effects of constraint variations and ductile tearing on (macroscopic) cleavage fracture toughness over a wide range of loading and crack configurations.*

Key words: *cleavage fracture, statistical effects, weakest link, local approach, Weibull stress*

1. INTRODUCTION

The fracture behavior of structural components subjected to various loading and environmental conditions is of obvious relevance in assessing structural integrity. The increasing demand for ensuring acceptable levels of structural safety has spurred a flurry of predictive methodologies aimed at quantifying the impact of defects in load-bearing materials such as, for example, cracks in critical weldments of high pressure vessels. Such methodologies play a key role in repair decisions and life-extension programs for in-service structures (e.g., aerospace, nuclear and offshore structures). While mechanical failures in structural members and components may result from a combination of several material degradation processes, assessments of structural integrity generally focus on cleavage fracture. This fracture mode potentially limit the load bearing capacity of the structure as local crack-tip instability may trigger catastrophic failure at low applied stresses with little plastic deformation.

Conventional fracture assessments of large engineering structures using laboratory specimen data most often employ a one-parameter characterization [1] of loading and toughness (K_I, J or CTOD, δ). The more recent two-parameter approaches (J-T [2-6] and J-Q [7, 8] methodologies) retain contact with traditional fracture mechanics and provide a concise framework to represent measured toughness values in terms of a J-T or J-Q fracture locus [38]. However, such methods are conservative (i.e., the failure of a cracked component at a given load is overpredicted) and do not provide a means to *predict* the effects of constraint variations and prior ductile tearing on toughness. Further, cleavage fracture is a highly localized, inherently random phenomenon which exhibits strong sensitivity to material characteristics at the microlevel. In particular, the random inhomogeneity in local features of the material causes large scatter in experimentally measured values of fracture toughness (K_{Ic}, J_c or CTOD) – see [38] for illustrative data. Such features make assessments of structural integrity using laboratory testing of standard specimens and simplified crack configurations a complex task: what is the "actual" material toughness and how is the scatter in measured values of fracture toughness incorporated in procedures for defect assessments?

There has recently been a surge of interest in analyzing and predicting material failure caused by transgranular cleavage based upon a probabilistic interpretation of the fracture process. A primary impetus for bringing probabilistic fracture mechanics concepts into play is the inherent random nature of fracture. Beremin [9], Wallin et al. [10-13], Lin et al. [14], Brückner et al. [17], Godse and Gurland [15] among others considered models of this type to provide a link between the size of carbides particles dispersed in the material and the inhomogeneous stress fields ahead of a macroscopic crack. The work of Beremin [9] attains particular relevance here as it introduced the Weibull stress (σ_w) as a suitable crack-tip parameter incorporating a local criterion for fracture. More recent efforts in this area have focused on developing transferability models for cleavage fracture toughness based upon the Beremin's Weibull stress. Bakker and Koers [37], Minami et al. [19], Ruggieri et al.[20], assess effects of specimen thickness and crack length on elastic-plastic fracture toughness (J_c, δ_c). Further studies by Ruggieri and Dodds [21-25] generalize the Weibull stress for stationary and growing cracks to include effects of loss of constraint and ductile tearing on macroscopic fracture toughness.

The objectives in developing probabilistic models to describe unstable crack propagation are essentially two fold. First, for a structure containing cracks of different sizes and subjected to complex loading histories, we seek to determine limiting distributions for the (local) fracture stress which couple remote loading (as measured by J or CTOD) with the operative fracture mechanism at the microlevel. In the context of probabilistic models, a fracture parameter associated with the limiting distribution then describes macroscopic fracture behavior for a wide range of loading conditions and crack configurations. As a second objective, we seek to predict unstable crack propagation in larger flawed structures on the basis of a probabilistic fracture parameter. Experimentally measured values of fracture toughness for one configuration (e.g., small laboratory specimens) are rationally extended to predict unstable crack propagation for other crack configurations, provided similarities in both limiting distributions for such a fracture parameter exist.

This study explores the development of a probabilistic (micromechanics) framework applicable to cleavage fracture to predict effects of constraint loss and ductile tearing on macroscopic fracture toughness. The presentation is given in three parts: Part I describes a probabilistic model employing the statistics of microcracks and a local failure criterion to link the microregime of fracture and macroscopic (remote) loading; Part II provides key features of the micromechanics approach in characterizing fracture behavior under small scale yielding (SSY) conditions [39]; the issue of parameter calibration and representative applications of the methodology are presented in Part III [40]. Specifically in Part I, the random nature of cleavage fracture due to inhomogeneity in the local characteristics of the material drives the development of a relationship to couple macroscopic fracture behavior with microscale events. For stress-controlled, cleavage mechanisms of material failure, the Weibull stress (σ_w) emerges as a probabilistic fracture parameter defining conditions leading to (local) fracture. This parameter permits predictions of the strong effects of constraint variations on (macroscopic) cleavage fracture toughness over a wide range of loading and crack configurations. This study and its sequels build upon previous work by Ruggieri and Dodds [21-23].

2. LIMITING DISTRIBUTION FOR THE FRACTURE STRESS IN 3-D

Cleavage fracture in low carbon, ferritic steels occurs primarily by the formation of microcracks at carbides in regions which undergo inhomogeneous plastic deformation [26-28]. These cracked carbides usually appear along grain boundaries and provide the cleavage nucleation sites. The present work adopts the viewpoint that cleavage fracture is a two-stage process: a) microcracks are generated due to localized and inhomogeneous plastic flow in a sufficiently stressed region of the material [28] and b) unstable crack propagation occurs when the local tensile stress acting on these microcracks reaches a critical tensile stress, σ_c [29]. Without making recourse to detailed metallurgical descriptions of the microscale fracture process, the near-tip stressed region ahead of a macroscopic crack or a notch depicted in Fig. 1(a) defines the *fracture process zone*; this region with size $5 \sim 10$ CTOD (δ) contains the potential sites for cleavage nucleation.

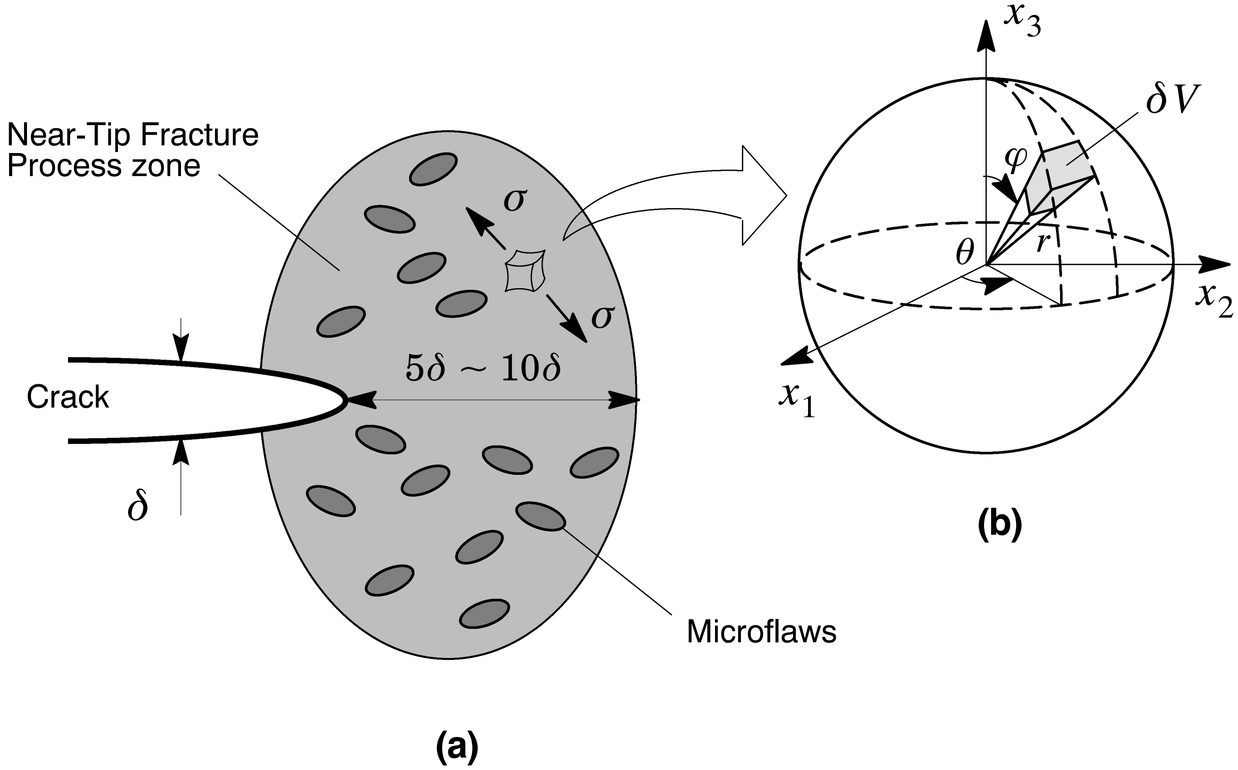

Figure 1 *(a) Fracture process zone ahead a macroscopic crack containing randomly distributed flaws; (b) Unit volume ahead of crack tip subjected to a multiaxial stress state.*

Development of a limiting distribution for the fracture stress of a multiaxially stressed cracked body begins by considering a *stationary* macroscopic crack lying in material containing randomly oriented microcracks (microflaws), uniformly distributed in location. Figure 1(b) illustrates an arbitrarily stressed, *unit* volume V near a crack or a notch; the stress state is represented by the principal stresses (σ_1, σ_2, σ_3). Two fundamental assumptions underlie the present probabilistic framework: (1) the fracture process zone near the crack tip consists of a large number of statistically independent, uniformly stressed, small volume elements, denoted δV, and (2) failure of this small volume element occurs when the size of a random flaw exceeds a critical size, i.e., $a > a_c$. Based upon probability theory, the well-known Poisson postulates (see, e.g., Feller [30]) provide two complementary assumptions: (1) failures occurring in non-overlapping volumes are statistically independent events and (2) the probability of failure for δV is proportional to its volume, i. e., $\delta \mathcal{P} = \mu \delta V$ when δV is sufficiently small. Here, the proportionality constant μ is the average number of flaws with size $a > a_c$ per unit volume. The elemental failure probability, $\delta\mathcal{P}$, is then related to the distribution of the largest flaw in a reference volume of the material, which can be expressed as

$$\delta\mathcal{P} = \delta V \int_{a_c}^{\infty} g(a)da \tag{1}$$

where $g(a)da$ defines the number of microcracks per unit volume having sizes between a and $a + da$.

Using a Taylor series expansion [31] of the exponential function e^x (with second-order terms neglected for sufficiently small x), the probability that no failure (probability of survival) will occur in the volume element becomes

$$1 - \delta\mathcal{P} = 1 - \delta V \int_{a_c}^{\infty} g(a)da = \exp\left[- \delta V \int_{a_c}^{\infty} g(a)da \right] + O(\delta V) \ . \tag{2}$$

Now, invoking weakest link arguments to derive the distribution of failure for the entire volume V (see Fig. 1), a "chain" analogy is readily established allowing proper interpretation of the resulting limiting distribution. Within this context, V is viewed as a chain consisting of n small elements δV so that failure of a single element leads to the collapse of the whole chain. The failure probability of V, expressed by $\mathcal{P}_0$, is then written in the form

$$\mathcal{P}_0 = 1 - \prod_{i=1}^{n} (1 - \delta\mathcal{P}_i) \ , \tag{3}$$

which is the familiar weakest link formulation applied to the volume V. Substituting Eq. (2) in the above Eq. (3) and working out the resulting expression with $n \to \infty$ (and $\delta V_i \to dV$), the failure probability of V becomes

$$\mathcal{P}_0 = 1 - \exp\left[- \int_V dV \int_{a_c}^{\infty} g(a)da \right] . \tag{4}$$

To arrive at a closed form for the failure probability of the unit volume V in terms of the near-tip stress field, an approximate description for the distribution of microcracks is required. A common assumption adopts an asymptotic distribution for the microcrack density, $g(a)$, in the form [32, 33]

$$g(a) = \frac{1}{V_0}\left(\frac{c_0}{a}\right)^{\xi} \ , \tag{5}$$

where ξ and c_0 are parameters of the distribution and V_0 denotes a reference volume. Now, the implicit distribution of fracture stress can be made explicit by introducing the dependence between the critical microcrack size, a_c, and stress in the form $a_c = (K^2/Y\sigma^2)$, where Y represents a geometry factor and σ denotes a *tensile* (opening) stress acting on the microcrack plane. Consequently, substituting Eq. (5) into Eq. (4) and working out the crack size integral yields the expression for $\mathcal{P}_0$ in the form

$$\mathcal{P}_0 = 1 - \exp\left[- \frac{1}{V_0} \int_V \left(\frac{\sigma}{\sigma_u}\right)^m dV \right] \tag{6}$$

where parameters $m = 2\xi - 2$ and σ_u define the microcrack distribution.

Employing the usual transformation of Cartesian coordinates (x_1, x_2, x_3) in spherical coordinates (r, θ, φ) by the mapping (see Fig. 1)

$$
\begin{aligned}
x_1 &= r \sin\varphi \cos\theta \\
x_2 &= r \sin\varphi \sin\theta \\
x_3 &= r \cos\varphi
\end{aligned} \tag{7}
$$

the limiting distribution of the fracture stress for the unit volume V at a given load level (conveniently represented by J in the present work) follows as

$$
\mathcal{P}_0(J) = 1 - \exp\left[-\frac{1}{4\pi V_0} \int_0^{2\pi} \int_0^{\pi} \left(\frac{\sigma}{\sigma_u} \right)^m \sin\varphi \, d\varphi \, d\theta \right] \tag{8}
$$

where the specific integration of the (tensile) stress over the curvilinear coordinates (θ, φ) includes the random orientation of microcracks. Since the reference volume, V_0, only scales $g(a)$ but does not change the distribution shape, it has no effect on m and is assigned a unit value for convenience in the computations. In the present work, the *active* fracture process zone is defined as the loci where $\sigma_1 \geq \lambda\sigma_0$, with $\lambda \approx 2$. Alternative definitions for the fracture process zone include the plastic region ahead of the macroscopic crack [9,16], $\sigma_e \geq \sigma_0$ where σ_e denotes the equivalent Mises stress.

Using again weakest link arguments, Eq. (8) can be generalized to any multiaxially stressed region, such as the fracture process zone ahead of a macroscopic crack or notch (see Fig. 1). Thus, the statistical problem of determining a limiting distribution for the fracture strength of the entire solid is equivalent to determining the distribution of the weakest unit volume V. The fundamental assumption is that the near-tip fracture process zone consists of N arbitrary and statistically independent, unit volumes V. Consequently, the failure probability of the cracked body when $N \to \infty$, denoted as $\mathcal{P}$, is given by

$$
\mathcal{P}(J) = 1 - \exp\left[-\frac{1}{4\pi V_0} \int_\Omega \int_0^{2\pi} \int_0^{\pi} \left(\frac{\sigma}{\sigma_u} \right)^m \sin\varphi \, d\varphi \, d\theta \, d\Omega \right] \tag{9}
$$

where Ω denotes the volume of the near-tip fracture process zone.

Equation (9) implicitly defines a zero threshold stress for fracture; consequently, stresses vanishingly small compared to the fracture stress will yield a non-zero (albeit small) probability for fracture. A more refined form for the limiting distribution for the fracture strength of a cracked solid can be given as

$$
\mathcal{P}(\sigma) = 1 - \exp\left[-\frac{1}{4\pi V_0} \int_\Omega \int_0^{2\pi} \int_0^{\pi} \left(\frac{\sigma - \sigma_{th}}{\sigma_u} \right)^m \sin\varphi \, d\varphi \, d\theta \, d\Omega \right] \quad , \quad \sigma \geq \sigma_{th} \tag{10}
$$

where σ_{th} is the threshold stress and has the physical interpretation of a lower bound strength for fracture. The failure probability for the cracked solid is zero for any stress below σ_{th}. However, because the threshold stress represents a lower bound strength at the microscale level, a "correct" value for σ_{th} is a somewhat elusive concept which raises the question of its significance in assessing the fracture behavior of flawed structures. Further, as shown by Ruggieri and Dodds [21], such refinement does not appear to provide significant improvements in predictions of the fracture behavior. Although the debate over a physically meaningful value for σ_{th} has obvious importance, we adopt the simplest form of the limiting distribution for the fracture stress by conveniently setting $\sigma_{th} = 0$ in Eq. (10). All subsequent results are equally valid for any $\sigma_{th} \geq 0$ (which should be adopted or known *a priori*) by simply defining $\sigma^* = \sigma - \sigma_{th}$.

3. THE WEIBULL STRESS FOR STATIONARY AND GROWING CRACKS

In the probabilistic framework adopted here, the introduction of a probabilistic fracture parameter plays a key role in the development of procedures that unify toughness measures across different crack configurations subjected to varying loading modes. Following the general development previously described, the Weibull stress (σ_w), a term coined by the Beremin group [9], is given by integration of the tensile stresses over the fracture process zone in the form

$$\sigma_w = \left[\frac{1}{4\pi V_0} \int_{\Omega} \int_0^{2\pi} \int_0^{\pi} \sigma^m \sin\varphi \, d\varphi \, d\theta \, d\Omega \right]^{1/m} , \tag{11}$$

from which the limiting distribution (9) can be rewritten as

$$\mathcal{P}(\sigma_w) = 1 - \exp\left[- \left(\frac{\sigma_w}{\sigma_u} \right)^m \right] . \tag{12}$$

Equation (12) defines a two-parameter Weibull distribution [34] in terms of the Weibull modulus m and the scale factor σ_u. Previous work [9, 19, 35] has shown that m takes a value in the range 10∼22 for typical structural steels.

The Weibull stress describes local conditions leading to unstable (cleavage) failure and appears, at least as a first approximation, to remain applicable during small amounts of ductile crack extension. Highly localized, non-planar crack extension and void growth at the larger inclusions, both of which occur over a scale of $\lesssim \delta_{Ic}$ (the CTOD at *onset* of crack growth initiation), should not alter the material properties m and σ_u over the much larger process zone relevant for cleavage initiation. Further, small amounts of ductile crack growth modify the stress history of material points within the process zone for cleavage fracture which affects directly the evolution of Weibull stress. A detailed discussion of the approach adopted here for generating the evolution of the Weibull stress with J (or equivalently CTOD) for a growing crack is given by Ruggieri and Dodds [21].

Figure 2 illustrates the development of the *active* fracture process zone (recall that the fracture process zone is defined as the loci where $\sigma_1 \geq \lambda\sigma_0$, with $\lambda \approx 2$) given by a snapshot of the stress field ahead of the growing crack. Points on such a contour all lie within the forward sector $|\theta| \leq \pi/2$. The envelope of all material points for which $\sigma_1 \geq \lambda\sigma_0$ during the history of growth defines an alternative, *cumulative* process zone. Consequently, the 3-D form of the Weibull stress for a growing crack becomes simply

$$\sigma_w = \left[\frac{1}{4\pi V_0} \int_{\Omega^*} \int_0^{2\pi} \int_0^{\pi} \sigma^m \sin\varphi \, d\varphi \, d\theta \, d\Omega^* \right]^{1/m} \tag{13}$$

where Ω^* denotes the active volume of the fracture process zone, $\sigma_1 \geq \lambda\sigma_0$, which moves forward with the advancing tip. The proposed generalization of σ_w to include ductile tearing maintains the relative simplicity of computations while, at the same time, fully incorporating the effects of alterations in the stress field ahead of the crack tip.

4. FINITE ELEMENT REPRESENTATION OF THE WEIBULL STRESS

This section briefly summarizes the finite element form of the Weibull stress expression for a stationary and a growing crack, Eq. (11) and Eq. (13), employed in numerical computations utilizing σ_w [22]. In parametric space, the current (deformed) Cartesian coordinates x_i of any point inside a 8-node tri-linear element are related to the parametric coordinates η_i through the relationship [36]

$$x_i = \sum_{k=1}^{8} N_k x_{ik} \quad , \quad i = 1, 2, 3 \tag{14}$$

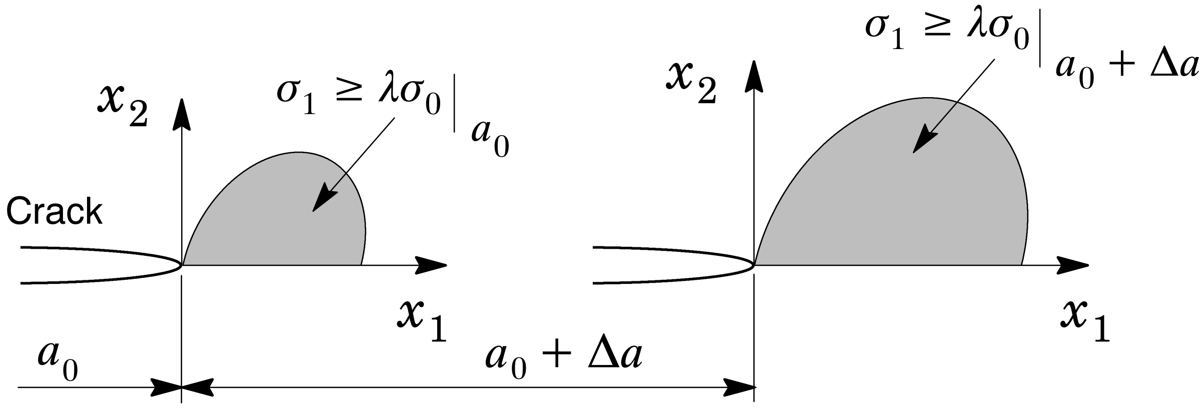

Figure 2 *Schematic representation for the evolution of the fracture process zone for a growing crack. The crack has advanced from* $a = a_0$ *to* $a = a_0 + \Delta a$.

where N_k are the shape functions corresponding to node k and x_{ik} are the current (deformed) nodal coordinates, $x_i = X_i + u_i$. The shape functions have standard form

$$N_k = \frac{1}{8}\prod_{i=1}^{3}(1 + \eta_i\eta_{ik}) \quad , \quad k = 1, \ldots, 8 \tag{15}$$

where η_{ik} denotes the parametric coordinates of node k.

Let $|J|$ denote the determinant of the standard coordinate Jacobian between deformed Cartesian and parametric coordinates. Then using standard procedures for integration over element volumes, the Weibull stress has the form

$$\sigma_w = \left[\frac{1}{4\pi V_0}\sum_{n_e}\int_{\Omega_e}\int_0^{2\pi}\int_0^{\pi}\sigma^m \sin\varphi d\varphi d\theta d\Omega_e\right]^{1/m} \tag{16}$$

$$= \left[\frac{1}{4\pi V_0}\sum_{n_e}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\int_0^{2\pi}\int_0^{\pi}\sigma^m |J| \sin\varphi d\varphi d\theta d\eta_1 d\eta_2 d\eta_3\right]^{1/m} \tag{17}$$

where n_e is the number of elements inside the fracture process zone near the crack tip and Ω_e is the volume of the element. The process zone used here includes all material inside the loci $\sigma_1 \geq \lambda\sigma_0$, with $\lambda = 2$. For computational simplicity, an element is included in the fracture process zone if the σ_1 computed at $\eta_1 = \eta_2 = \eta_3 = 0$ exceeds $2\sigma_0$.

Application of Eq. (17) requires a specific definition for the tensile stress, σ, acting on the microcrack. This tensile stress can be determined for each pair of coordinates (θ, φ) by adopting a convenient fracture criterion coupled with a geometric shape for the microcrack [18,22]. However, little agreement exists about which criterion most effectively describes cleavage fracture. Using the simple, maximum principal tensile stress criterion to describe unstable crack propagation, the Weibull stress takes the form

$$\sigma_w = \left[\frac{1}{V_0} \sum_{n_e} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \sigma_1^m \, | J | \, d\eta_1 d\eta_2 d\eta_3 \right]^{1/m} \tag{18}$$

which reflects the independence of the principal stress on the curvilinear coordinates (θ, φ). This expression for the Weibull stress represents the integral form in parametric space of Beremin's formulation [9].

5 CONCLUDING REMARKS

We have presented a probabilistic-based framework to predict the effects of constraint loss and ductile tearing on macroscopic measures of cleavage fracture toughness (J_c, δ_c) applicable for ferritic materials in the ductile-to-brittle transition region. To model the statistics of microcracks and the pronounced effects on scatter of measured J_c -values in the transition region, we employ the Weibull stress, σ_w, as a near-tip, or *local,* fracture parameter; unstable crack propagation occurs when σ_w attains a critical value. Both constraint loss and ductile tearing affect the evolution of σ_w under increasing applied J in common fracture test specimens. Consequently, this parameter permits predictions of the strong effects of constraint variations and ductile tearing on (macroscopic) cleavage fracture toughness over a wide range of loading and crack configurations. The predictive capability of the micromechanics (probabilistic) framework is explored in Parts II [39] and III [40] of this study.

Acknowledgements

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