WSTRESS

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Numerical Evaluation of Probabilistic Fracture Parameters for 3-D Cracked Solids and Calibration of Weibull Stress Parameters

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Nessun effetto è in natura sanza ragione, intendi la ragione e non ti bisogna sperienza

There is no result in nature without a cause; understand the cause and you will have no need of the experiment.

Leonardo da Vinci, In Codice Atlantico, 1518

Abstract

This document describes the theoretical aspects and commands necessary to use ***WSTRESS***, a research code for computation of probabilistic fracture parameters applicable to 3-D cracked solids based upon a micromechanics (local) approach incorporating the statistics of microcracks. ***WSTRESS*** computes the Weibull stress, σ_w, as well as its modified form, $\tilde{\sigma}_w$, and performs the calibration of the Weibull parameters from fracture mechanics test data. Recent developments have focused on analyzing the effects of constraint loss on macroscopic measures of cleavage fracture toughness (J_c, δ_c). These efforts provided ***WSTRESS*** with key capabilities to address the strong effects of constraint on cleavage fracture behavior and to incorporate effects of plastic strain on cleavage fracture toughness in a probabilistic framework. On-going work continues to provide ***WSTRESS*** with additional capabilities to support other engineering-level applications in fracture assessments of cracked solids and structural components containing crack-like flaws.

WSTRESS implements a simple form of the weakest link model applicable to 3-D cracked solids under arbitrary loading conditions. Effects of local inhomogeneity and random characteristics of the material at the microscale level are included by using the asymptotic theory of extreme values to describe the distribution of flaw size in the material. Further, the methodology couples the (stress-strain) loading history in the near-tip region where fracture takes place with the (operative) microstructural fracture mechanism. The Weibull stress (σ_w) then emerges as a *probabilistic* fracture parameter reflecting the local damage of material near the crack tip. Hence, overall fracture conditions in a specimen or structural component may be described by evolution of this micromechanistically based parameter with the macroscopic loading, defined conveniently by J or CTOD (δ). The formulation currently implemented in ***WSTRESS*** conveniently handles the inhomogeneous character of the near-tip stress fields and computes the Weibull stress by integration of the local tensile stresses using a numerical scheme at the element level. As a further capability, the methodology implemented in ***WSTRESS*** also enables incorporation of effects of near-tip plastic strain on cleavage microcracking which impacts directly the magnitude of the Weibull stress and, consequently, the toughness scaling correction.

WSTRESS takes input commands to define the numerical (finite element) model, solution parameters, experimental toughness data and output requests in a format-free, English-like structure from a user-specified input file. This input file may include extensive user comments and is thus self-documenting. Finite element results required to compute the Weibull stress consist of displacements, stresses and strains in standard Patran format (binary or ascii) written directly by the finite element code WARP3D.

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Summary

1

Introduction

1.1 Local Approaches to Cleavage Fracture

The increased demand for more accurate structural integrity and fitness-for-service (FFS) analysis of a wide class of engineering structures, including nuclear reactor pressure vessels, piping systems and storage tanks, has stimulated renewed interest in advancing current safety assessment procedures of critical structural components, including life-extension programs and repair decisions of aging structures. Simplified fracture mechanics based approaches for quantitative analysis of material degradation, as of interest in assessments of crack-like flaws formed during in-service operation, focus primarily on the potential for catastrophic failure due to low toughness behavior. Specifically for ferritic materials at temperatures in the ductile-to-brittle transition (DBT) region, such as carbon and low-alloy steels typically used in many structural applications, unstable fracture by transgranular cleavage still represents one of the most serious failure modes as local crack-tip instability may trigger catastrophic structural failure at low applied stresses with little plastic deformation. These methods, also referred to as engineering critical assessment (ECA) procedures, rely on direct application of macroscopic measurements of cleavage fracture toughness (such as the J-integral at cleavage instability, J_c, or the critical Crack Tip Opening Displacement, CTOD or δ_c) derived from conventional fracture specimens tested under high constraint conditions, similar to those of small-scale yielding (SSY), to define conservative flaw acceptance criteria. While conventional ECA methodologies clearly simplify integrity assessments of in-service structural components, they have limited ability to predict the potential strong influence of constraint on fracture behavior and, perhaps more importantly, do not address the strong sensitivity of cleavage fracture to material characteristics at the microlevel.

The early recognition of these limitations prompted a surge of interest in analyzing, predicting and unifying toughness measures across different crack configurations and loading modes based on a micromechanics interpretation of the cleavage fracture process. Here, attention has been primarily focused on probabilistic models incorporating weakest link statistics, most often referred to as local approaches to fracture (LAF) [1, 2, 3], to describe material failure caused by transgranular cleavage for a wide range of loading conditions and crack geometries. In the context of probabilistic fracture mechanics, the methodology yields a limiting distribution that describes the coupling of the (local) fracture stress with remote loading (as measured by J or CTOD) in terms of a fracture parameter characterizing macroscopic fracture behavior for a wide range of loading conditions and crack configurations. Among these earlier research efforts, the seminal work of the French group Beremin [1] provided the impetus for the development of a framework establishing a relationship between the microregime of fracture and macroscopic crack driving forces (such as the J-integral) by introducing the Weibull stress (σ_w) as a probabilistic fracture parameter directly connected to the statistics of microcracks (weakest link philosophy). A key feature of this methodology is that σ_w incorporates both the effects of stressed volume (the fracture process zone) and the potentially strong changes in the character of the near-tip stress fields due to constraint loss, thereby providing the necessary framework to correlate fracture toughness for varying crack configurations under different loading (and possibly temperature and strain rate) conditions. Previous research efforts to develop a transferability model to elastic-plastic fracture toughness values rely on the notion of the Weibull stress as a crack-tip driving force [4, 5, 6, 7] by adopting the simple axiom that unstable crack propagation (cleavage) occurs at a critical value of the Weibull stress, $\sigma_{w,c}$.

Several other approaches along these lines have been proposed to relate local failure conditions with macroscopic fracture parameters and to the subsequent prediction of toughness *loci*. For the transgranular cleavage mechanism of ferritic steels, a number of such models explicitly adopt weakest link arguments that yield statistical functions reflecting the inhomogeneous character of near-tip stresses [1, 8, 9, 10]. Similar statistical approaches falling within the scope of micromechanics methodologies have also been described by Wallin, et al. [11, 12, 13, 14], Lin et al. [15], Mudry [2], Brückner, et al. [16, 17], Minami et al. [18], Koers et al. [19], Ruggieri et al. [20], among others. Recent transferability models for elastic-plastic fracture toughness values employing the Weibull stress approach [4, 5, 21, 22, 23, 24] have proven effective to predict constraint and specimen geometry effects on measured distributions of fracture toughness values for structural steels. Under increased remote loading (as measured by J or, equivalently, CTOD), differences in evolution of the Weibull stress reflect the potentially strong variations, including 3-D effects, of near-tip stress fields due to constraint loss while, at the same time, incorporating statistical effects of the material microstructure on toughness. The procedure is thus capable of correcting measured distributions of toughness values for fracture specimens and structural components with different geometry and loading conditions based on a relatively simple application of the toughness scaling methodology phrased in terms of the evolution of σ_w *vs.* the loading parameter, most often conveniently characterized in terms of the J-integral.

1.2 What is *WSTRESS*

This document describes the theoretical aspects and commands necessary to use ***WSTRESS***, a research code for computation of probabilistic fracture parameters applicable to 3-D cracked solids based upon a micromechanics (local) approach incorporating the statistics of microcracks. ***WSTRESS*** computes the Weibull stress, σ_w, as well as its modified form, $\tilde{\sigma}_w$, and performs the calibration of the Weibull parameters from fracture mechanics test data. It is based on previous research efforts [4, 5, 21, 22, 23, 24] to analyze the effects of constraint loss on macroscopic measures of cleavage fracture toughness (J_c, δ_c). These efforts provided ***WSTRESS*** with key capabilities to address the strong effects of constraint on cleavage fracture behavior and to incorporate effects of plastic strain on cleavage fracture toughness in a probabilistic framework. On-going work continues to provide ***WSTRESS*** with additional capabilities to support other engineering-level applications in fracture assessments of cracked solids and structural components containing crack-like flaws.

WSTRESS implements a simple form of the weakest link model applicable to 3-D cracked solids under arbitrary loading conditions. Effects of local inhomogeneity and random characteristics of the material at the microscale level are included by using the asymptotic theory of extreme values [25, 26] to describe the distribution of flaw size in the material. Further, the methodology couples the (stress-strain) loading history in the near-tip region where fracture takes place with the (operative) microstructural fracture mechanism. The Weibull stress (σ_w), a term coined by the Beremin group [1], then emerges as a *probabilistic* fracture parameter reflecting the local damage of material near the crack tip. Hence, overall fracture conditions in a specimen or structural component may be described by evolution of this micromechanistically based parameter with the macroscopic loading, defined conveniently by J or CTOD (δ). The formulation currently implemented in ***WSTRESS*** conveniently handles the inhomogeneous character of the near-tip stress fields and computes the Weibull stress by integration of the local tensile stresses using a numerical scheme at the element level. As a further capability, the methodology implemented in ***WSTRESS*** also enables incorporation of effects of near-tip plastic strain on cleavage microcracking which impacts directly the magnitude of the Weibull stress and, consequently, the toughness scaling correction.

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This manual is organized as follows. Chapter 2 provides the theoretical background related to probabilistic modeling of cleavage fracture which has a direct bearing on the probabilistic methodology employed in ***WSTRESS*** and on the Weibull stress model addressed in Chapter 3, including effects of plastic strain on cleavage fracture. Chapter 4 presents details of the calibration procedure implemented in the code to determine the Weibull modulus, m, using two sets of fracture toughness data. Chapters 5-6 describe the commands and input data needed for execution of ***WSTRESS***. Chapter 7 presents an illustrative example using fracture toughness data for an A285 Gr C pressure vessel steel which serves as a prototype for calibrating the Weibull stress parameter, m, for a cracked or notched structure. Appendix A provides details of point estimation for the Weibull parameters using the maximum likelihood method.

2

Probabilistic Modeling of Cleavage Fracture

The framework presented here addresses the problem of relating the macroscopic fracture toughness of cracked structures, as measured by the J-integral or the crack-tip opening displacement, (CTOD or δ), to a micromechanics model for cleavage fracture. This type of fracture has obvious significance in assessing the structural integrity of engineering components as it often leads to catastrophic failure at low applied stresses with little plastic deformation. One of the primary interests focuses on the transferability of fracture toughness data obtained from relatively simple laboratory testing of small (standard) specimens to structural components. Here, substantial progress has been made in recent years in characterizing and analyzing the fracture problem from a phenomenological viewpoint of unstable crack propagation. Assessments of fracture behavior generally employ a conventional one-parameter characterization [29] or the more recent two-parameter characterization of crack-tip stress and deformation fields, such as the J-T [30, 31, 32, 33, 34] and J-Q [35, 36] approaches, as well as higher-order asymptotic descriptions of crack-tip fields [37, 38, 39, 40, 41, 42].

However, cleavage fracture is a highly localized phenomenon which exhibits strong sensitivity to material characteristics, structure geometry and loading history. In particular, the random inhomogeneity in local features of the material causes large scatter in measured fracture toughness data. Consequently, realistic methodologies for fracture assessments of engineering components must adopt a probabilitic, rather than a deterministic, treatment of fracture. In particular, probabilistic approaches employing local fracture criteria appear well suited to the task of describing overall conditions for cleavage fracture; such approaches couple the random nature of local failure with the (stress-strain) loading history in the near-tip region where fracture takes place.

In the present work, 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. The proposed framework considers a micromechanics model that employs the statistics of microcracks applicable for ferritic steels in the transition region. This model provides a connection between the microregime of failure and a tractable mathematical formulation within a continuum framework of fracture. Here, the underlying assumption, which appears most compatible with the physical process, is that there exist small, but finite, volumes of materials which fully embody a population of uniformly distributed flaws; their size and density constitute properties of the material. The resulting framework therefore reduces the brittle fracture problem to one of finding a critical flaw or, in general, of determining (implicitly) the extreme value distribution of flaw size in which weakest link arguments yield a statistical function describing overall fracture conditions in the specimen or structure. For stress-controlled cleavage mechanisms of material failure, the Weibull stress, σ_w, emerges as a fracture parameter defining the conditions leading to (local) fracture (see, e.g., Ruggieri and Dodds [4, 21, 43, 44], Gao et al. [24] and, more recently, Ruggieri [5, 45]).

The methodology implemented in ***WSTRESS*** does not attempt to generate the Weibull stress for the material based upon the actual microcrack distribution (such as measured by, for example, fractographic characterization of fracture-initiation particles dispersed into the ferrite matrix os structural steels). Without making recourse to detailed metallurgical measurements, ***WSTRESS*** constructs a relationship between the Weibull stress and macroscopic loading (as measured by J or CTOD) based upon an *ad-hoc* assumption for the microcrack distribution which is consistent with extreme value theory [46, 25, 47, 48]. While this procedure lacks a rigorous description of some material characteristics at the microscale level, it simplifies considerably the statistical treatment of fracture while, at the same time, yielding robust parameters for failure assessments of structures.

The next sections address the essential features of the probabilistic modeling of cleavage fracture needed to construct a toughness scaling methodology based on the Weibull stress concept. Attention is directed to the micromechanics of transgranular cleavage fracture in connection to a probabilistic interpretation of cleavage failure at the microlevel based on the statistics of microcracks.

2.1 Micromechanics of Transgranular Cleavage Fracture

This section reviews basic features of the transgranular cleavage fracture in polycrystalline metals; this failure mode most often occurs in *bcc* metals (e.g., low carbon steels) at low temperatures. A substantial number of studies and experimental observations have provided detailed descriptions of the cleavage fracture process [49, 50, 51, 52]. It is beyond the scope of the present report to survey all the work conducted on cleavage fracture and associated micromechanisms. However, some general and simple concepts needed to support the fracture methodology described in the following sections are briefly introduced.

Cleavage fracture occurs when a crack propagates unstably through a solid under tensile stress; the fracture of the material occurs simply by direct separation along preferred cleavage planes due to rupture of atomic bonds. The pioneering work of Griffith [53] recognized the fundamental importance of inherent microcracks in the material. These microcracks represent the precursors to fracture initiation and eventually produce stress concentration of sufficient magnitude to cause material separation at the microlevel. While the physical significance of this model is apparent, further consideration of how cleavage cracks form and their role in controlling fracture toughness of metals is needed to support the probabilistic framework for cleavage fracture based on the Weibull stress concept described next in Chapter 3.

Early progress in understanding the mechanisms of cleavage fracture in mild steels was achieved by means of detailed metallographic observations of cleavage microcracks. A number of works, including those of Low [54], Owen et al. [55], McMahon and Cohen [56] and Smith [51], revealed the formation of Griffith-like microcracks after the onset of yielding and localized plasticity primarily by the cracking of carbides along grain boundaries. This process occurs over one or two grains of the polycrystalline aggregate; once a microcrack has formed in a grain and spread through the nearby ferrite grain boundaries, it likely propagates with no significant increase in the applied stress unless the microcrack is arrested at the grain boundary [52]. A connection between fracture resistance and microestructure can be made by rationalizing the interdependence between microcrack nucleation and unstable propagation as illustrated schematically in Fig. 2.1: 1) fracture of a carbide particle assisted by plastic deformation of the surrounding matrix nucleates a Griffith-like microcrack; 2) the nucleated microcrack advances rapidly into the interior of the ferrite grain until it reaches a grain boundary and 3) fracture occurs when the microcrack is not arrested at a grain boundary barrier and thus propagates unstably. In terms of the Griffith cleavage criterion [53], the last condition means that the Griffith fracture energy to propagate the microcrack is larger than the specific surface energy of the grain boundary [52].

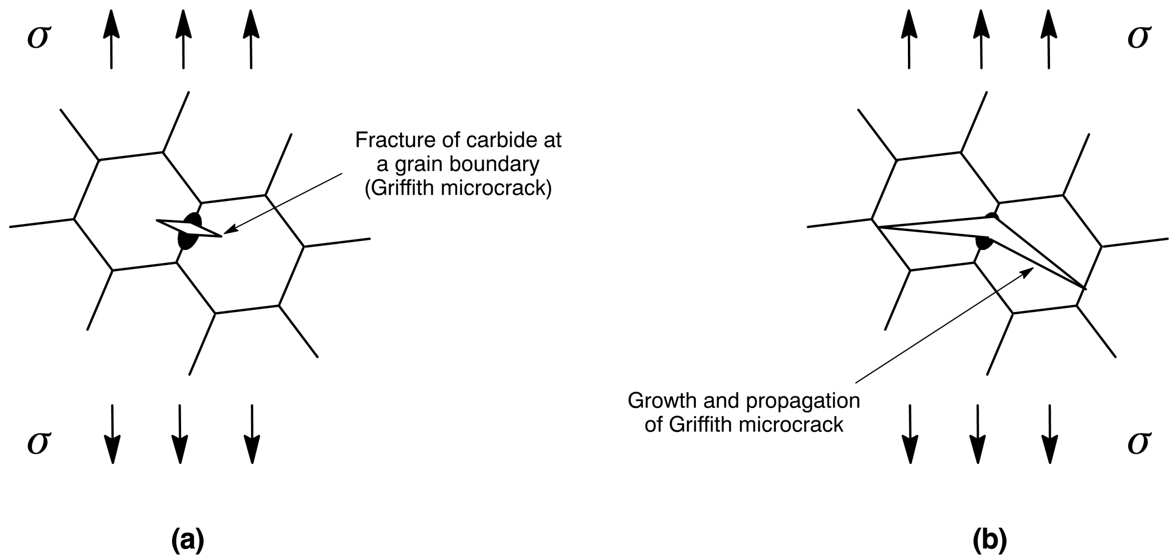

Figure 2.1: *Schematic process of cleavage fracture due to cracking of carbides at grain boundaries of ferritic steels: a) Fracture of carbide and formation of a Griffith-like microcrack; b) Growth of the Griffith microcrack into adjacent grains.*

In adopting the previous viewpoint of cleavage fracture in structural steels as controlled by the (critical) extension of Griffith-type microcracks across microstructural boundaries, it becomes apparent that fracture resistance depends on the local distribution of microcrack size and orientation. Consequently, the Griffith cleavage condition is met by the largest eligible microcrack present in a highly stressed volume with size of the order of a small multiple of the average grain diameter [52]. Such features require a more detailed formulation to describe the fracture behavior including a statistical analysis for the potential contributions of all eligible microcracks coupled with the extent of the highly stressed material rather than solely the magnitude of the stresses acting on the microcrack as will be addressed in Chapter 3.

2.2 Statistical Description of Cleavage Fracture Toughness Data

Experimental studies consistently reveal large scatter in the measured values of cleavage fracture toughness for ferritic steels tested in the DBT region. The connection between the local (cleavage) fracture process and extreme value statistics plays the key role in describing the scatter in fracture toughness values. A continuous probability function derived from weakest link statistics [47, 48, 57] conveniently characterizes the distribution of toughness values in the form [12, 26, 58]

$$F(J_c) = 1 - \exp\left[-\left(\frac{J_c - J_{min}}{J_0 - J_{min}}\right)^{\alpha}\right] \tag{2.1}$$

which is a three-parameter Weibull distribution with parameters (α, J_0, J_{min}). Here, α denotes the Weibull modulus (shape parameter), J_0 defines the characteristic toughness (scale parameter) and J_{min} is the threshold fracture toughness (*i.e.*, $F(J_c) = 0$ for $J_c \leq J_{min}$). Often, the threshold fracture toughness, J_{min}, is set equal to zero so that the Weibull function given by Eq. (2.1) assumes its more familiar two-parameter form

$$F(J_c) = 1 - \exp\left[-\left(\frac{J_c}{J_0}\right)^{\alpha}\right] \quad . \tag{2.2}$$

The above limiting distribution remains applicable for other measures of fracture toughness, such as K_{Jc} or CTOD (δ). A central feature emerging from the probabilistic treatment of brittle fracture based upon the weakest link statistics is that, under small scale yielding (SSY) conditions, the scatter in cleavage fracture toughness data is characterized by $\alpha = 2$ for J_c-distributions (δ_c-distributions) or $\alpha = 4$ for K_{Jc}-distributions [12, 18, 59]. Further examination of the statistical character for the toughness distribution under SSY conditions described by previous Eq. (2.2) is deferred to Section 3.6.

2.3 Statistics of Microcracks and Elemental Cleavage Failure Probability

To introduce a probabilistic treatment for arbitrarily stressed, 3-D crack configurations, research efforts have focused on probabilistic models which couple the micromechanical features of the fracture process (such as the inherent random nature of cleavage fracture) with the inhomogeneous character of the near-tip stress fields. Motivated by the specific micromechanism of transgranular cleavage, a number of such models (most often referred to as *local approaches*) employ weakest link arguments to describe the failure event. The overall fracture resistance is thus controlled by the largest fracture-triggering particle that is sampled in the fracture process zone ahead of crack front. Figure 2.2 defines the fracture process zone as the near-tip stressed region ahead of a macroscopic crack; this region with size $5 \sim 10\times$CTOD (δ) contains the potential sites for cleavage nucleation. The statistics of microcracks then provides a connection between the microregime of fracture and macroscopic (global) behavior which yields a statistical distribution for the (cleavage) fracture stress.

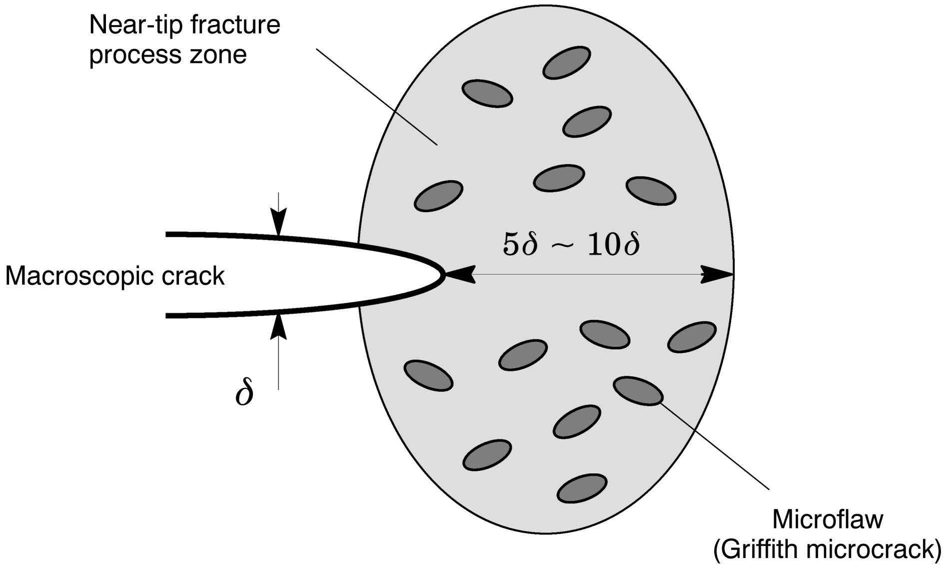

Figure 2.2: *Fracture process zone ahead a macroscopic crack containing randomly distributed Griffith-like microflaws.*

Development of a probabilistic model for cleavage fracture begins by introducing a limiting distribution for the fracture stress of a cracked body subjected to an arbitray stress state, where a stationary macroscopic crack lies in material containing randomly oriented microcracks (flaws), uniformly distributed in location. Figure 2.3 illustrates an arbitrarily stressed, unit volume V near a crack or a notch; the stress state is characterized by the principal stresses (σ_1, σ_2, σ_3). The fracture process zone near the crack tip is idealized as consisting of a large number of statistically independent, uniformly stressed, small volume elements, denoted δV. For definiteness, assume that failure of this small volume element occurs when the size of a random flaw exceeds a critical

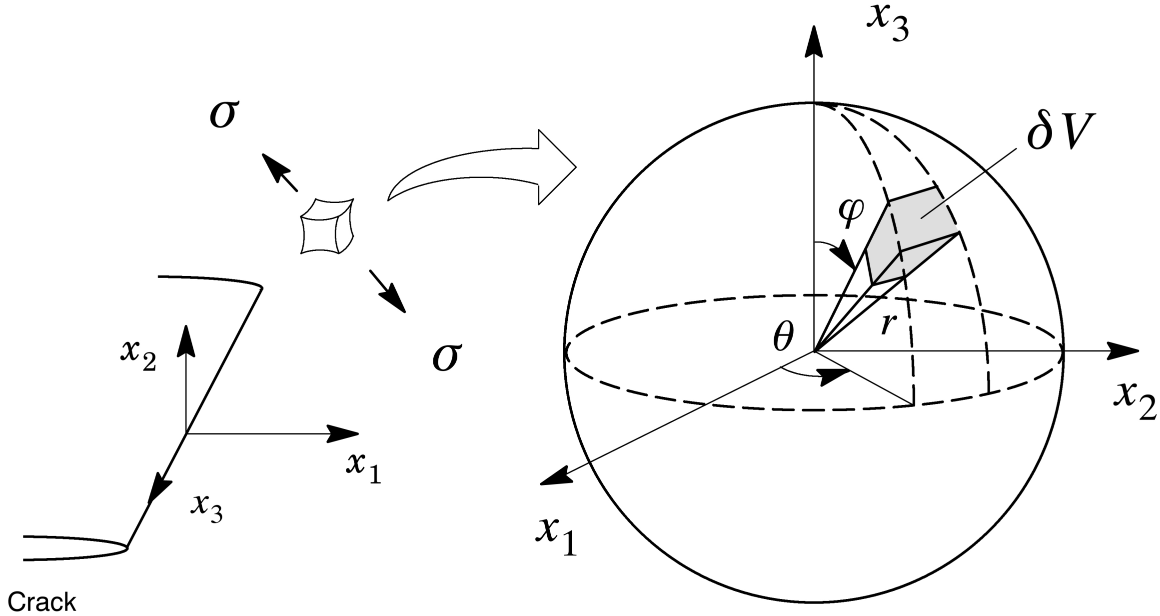

Figure 2.3: *Unit volume ahead of crack tip subjected to a multiaxial stress state.*

size, *i.e.*, $a > a_c$. Two fundamental assumptions based upon probability theory and the well-known Poisson postulates (see, *e.g.*, Feller [60]) underlie the present framework: (1) failures occurring in nonoverlapping volumes are statistically independent events and (2) the probability of failure for δV is proportional to its volume, *i. e.*, $\delta p = \mu \delta V$ when δV is small. Here, the proportionality constant μ can be interpreted as the average number of flaws with size $a \geq a_c$ per unit volume. The elemental failure probability, δp, is then related to the distribution of the largest flaw in a reference volume of the material, which can be expressed as

$$\delta p = \delta V \int_{a_c}^{\infty} g(a) da \tag{2.3}$$

where $g(a)da$ defines the number of microcracks per unit volume having sizes between a and $a+da$. Thus, the probability that no failure (probability of survival) will occur in the volume element becomes

$$1 - \delta p = 1 - \delta V \int_{a_c}^{\infty} g(a) da = \exp\left[-\delta V \int_{a_c}^{\infty} g(a) da\right] \tag{2.4}$$

which follows from a Taylor series expansion [61] of the exponential function in the form

$$e^{-x} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!} \tag{2.5}$$

with second-order terms neglected for sufficiently small x.

Using now weakest link arguments to derive the distribution of failure for the entire unit volume V (see Fig. 2.3), a "chain" analogy is readily established allowing proper interpretation of the resulting limiting distribution. Here, V is viewed as a chain consisting of n small elements so that failure of a single element leads to the failure of the whole chain. Following Freudenthal [48], the problem of the distribution of the weakest link is equivalent to that of the distribution of smalles values in samples of size n. Thus, if the fracture strength of the unit volume is determined by the local strength of its weakest volume element, the statistical distribution of the fracture strength is obtained in terms of the asymptotic theory of extreme values [25, 62] to describe the distribution of the smallest local strength for n volume elements.

The probability that all values in a sample of size n of a continuous random variable X with cumulative distribution $F(x)$ are less than x may be interpreted as the probability $\Phi_n(x)$ that x is the smallest among these values. Consequently, it follows from the multiplication rule that

$$\Phi_n(x) = 1 - [1 - F(x)]^n \quad . \tag{2.6}$$

Since the cumulative distribution, $F(x)$, in the above expression represents the elemental failure probability, δp, and, further, making $\Phi_n(x)$ as the failure probability of the unit volume, V, which is expressed by p_0, Eq. (2.6) can be rewritten as

$$p_0 = 1 - \prod_{i=1}^{n}(1 - \delta p_i) \tag{2.7}$$

which is the familiar weakest link formulation applied to the unit volume V. Substituting Eq. (2.4) in the above Eq. (2.7) yields

$$p_0 = 1 - \prod_{i=1}^{n} \exp\left[-\delta V_i \int_{a_c}^{\infty} g(a)da\right] = 1 - \exp\left[-\sum_{i=1}^{n} \delta V_i \int_{a_c}^{\infty} g(a)da\right] \quad . \tag{2.8}$$

Consequently, when $n \to \infty$ (and $\delta V \to dV$), Eq. (2.8) becomes

$$p_0 = 1 - \exp\left[-\int dV \int_{a_c}^{\infty} g(a)da\right] \quad . \tag{2.9}$$

To arrive at a closed form for the failure probability of the unit volume V in terms of the near-tip stress fields, 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 [48, 57]

$$g(a) = \frac{1}{V_0}\left(\frac{\zeta_0}{a}\right)^{\zeta} \tag{2.10}$$

where ζ_0 and ζ 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 $a_c = K_{Ic}^2/(Y\,\sigma_{eq}^2)$, where K_{Ic} is the material's fracture toughness, Y represents the specimen dependent geometry factor and σ_{eq} denotes an *equivalent* (effective) tensile (opening) stress acting on the microcrack plane. Consequently, substituting Eq. (2.10) into Eq. (2.9) and working out the crack size integral yields the expression for p_0 in the form

$$p_0 = 1 - \exp\left[-\frac{1}{V_0}\int_V \left(\frac{\sigma_{eq}}{\sigma_u}\right)^m dV\right] \tag{2.11}$$

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

The above development corresponds to a uniform distribution of microcracks inside the near-tip fracture process zone and, thus, does not consider their potential random orientation. Here, for a given microcrack position ahead of crack tip defined by the radius, r, the microcrack plane can be oriented according to different orientations defined by the angular coordinates (θ, φ), in which case the integral of Eq. (2.11) would be expressed as

$$p_0 = 1 - \exp\left[-\frac{1}{V_0}\int_0^r \int_0^{2\pi} \int_0^{\pi} \left(\frac{\sigma_{eq}}{\sigma_u}\right)^m r^2 \sin\varphi dr d\varphi d\theta\right] \quad . \tag{2.12}$$

where the usual transformation of Cartesian coordinates (x_1, x_2, x_3) into spherical coordinates (r, θ, φ) was employed by the mapping (see Fig. 2.3)

$$x_1 = r\sin\varphi\cos\theta \tag{2.13}$$

$$x_2 = r\sin\varphi\sin\theta \tag{2.14}$$

$$x_3 = r\cos\varphi \tag{2.15}$$

so that the equivalent stress, $\sigma_{eq,}$can now incorporate the combined effects of shear and tensile stresses acting on the microcrack plane. While Eq. (2.12) represents a more refined form of the failure probability of the unit volume V, it does not provide significant improvements in the predictive capability of the Weibull stress approach described next while, at the same time, adding more complexity and computational effort since a convenient fracture criterion and microcrack geometry must be specified at the onset of the analysis. Future versions of ***WSTRESS*** will implement the capability to treat the random orientation of microcracks and different fracture criteria incorporating the combined effects of shear and tensile stresses on σ_{eq}.

3

The Weibull Stress Model

3.1 The Weibull Stress for Cracked Solids

Using again weakest link arguments, the previous Eq. (2.11) can be generalized to any arbitrarily stressed region, such as the fracture process zone ahead of a macroscopic crack or notch illustrated in previous Fig. 2.2). 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 failure probability for 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, denoted as P_f, of a cracked body under a given remote loading, as characterized by the J-integral, is given by

$$P_f(J) = 1 - \prod_{j=1}^{N} [1 - p_{0,j}(J)] \tag{3.1}$$

which for $N \to \infty$ yields

$$P_f(J) = 1 - \exp\left\{ -\frac{1}{V_0} \int_\Omega \left[\frac{\sigma_{eq}(J)}{\sigma_u} \right]^m d\Omega \right\} \tag{3.2}$$

where Ω denotes the volume of the near-tip fracture process zone. In the present work, the *active* fracture process zone is defined as the loci where $\sigma_1 \geq \Lambda\sigma_{ys}$, in which σ_1 is the maximum principal stress acting on the unit volume, V, and σ_{ys} defines the material yield (reference) stress. Here, a value of $\Lambda \approx 2$ is most often adopted. The above expression remains applicable for other measures of remote loading, such as the CTOD or K_J.

Following this general development and omitting the dependence of σ_{eq} on the J-integral for clarity, the Weibull stress, σ_w, a term coined by the Beremin group [1], is given by integration of the equivalent tensile stresses over the fracture process zone in the form

$$\sigma_w = \left[\frac{1}{V_0} \int_\Omega \sigma_{eq}^m d\Omega \right]^{1/m} \tag{3.3}$$

from which the limiting distribution for the fracture stress defined by Eq. (3.2) now takes the form

$$P_f(\sigma_w) = 1 - \exp\left[-\left(\frac{\sigma_w}{\sigma_u}\right)^m\right] \quad . \tag{3.4}$$

The above Eq. (3.4) defines a two-parameter Weibull distribution [26, 58, 63, 64] in terms of the Weibull modulus, m, and the scale factor, σ_u. Previous works [1, 4, 5, 18, 45] have shown that m takes a value in the range $10 \sim 22$ for typical structural steels.

In the context of probabilistic fracture mechanics, the Weibull stress, σ_w, emerges as a near-tip parameter to describe the coupling of remote loading with a micromechanics model which incorporates the statistics of microcracks (weakest link philosophy). Unstable crack propagation (cleavage) occurs at a critical value of σ_w; under increased remote loading (J, CTOD or K_J), differences in evolution of the Weibull stress reflects the potentially strong variations of near-tip stress fields due to the effects of constraint loss.

3.2 Cleavage Fracture Criterion

For the general problem of a microcrack under combined loading, the local stress state may exhibit all three modes of deformation (I, II and III) illustrated in Fig. 3.1. Assuming that microcrack extension occurs without causing a significant readjustment in the surrounding stress field, a fracture criterion based upon the stress field existing just before the onset of unstable fracture is often adopted, in which an equivalent stress, σ_{eq}, drives the unstable propagation of the microcrack under an equivalent Mode I loading. The Weibull stress given by Eq. (3.3) then follows by integration of σ_{eq} over the fracture process zone.

While several criteria have been proposed to evaluate the critical stress at which the crack becomes unstable, ***WSTRESS*** currently uses a simplified criterion to describe cleavage fracture. Consistent with the critical stress theory underlying the present methodology, the present version of ***WSTRESS*** implements the maximum principal stress criterion briefly described next. Future versions of ***WSTRESS*** will implement other fracture criteria, such as the coplanar energy release rate criterion [65] most often adopted in the multiaxial form of σ_w - refer to the discussion at the end of Section 2.3.

3.2.1 Maximum Principal Stress Criterion

A convenient definition for the Weibull stress follows from the maximum principal stress criterion so that the equivalent tensile stress, σ_{eq}, is taken as the maximum principal stress, σ_1; here, the principal stress acts on all material points at the element. Here, the Weibull stress simply yields

$$\sigma_w = \left[\frac{1}{V_0}\int_\Omega \sigma_1^m d\Omega\right]^{1/m} \quad . \tag{3.5}$$

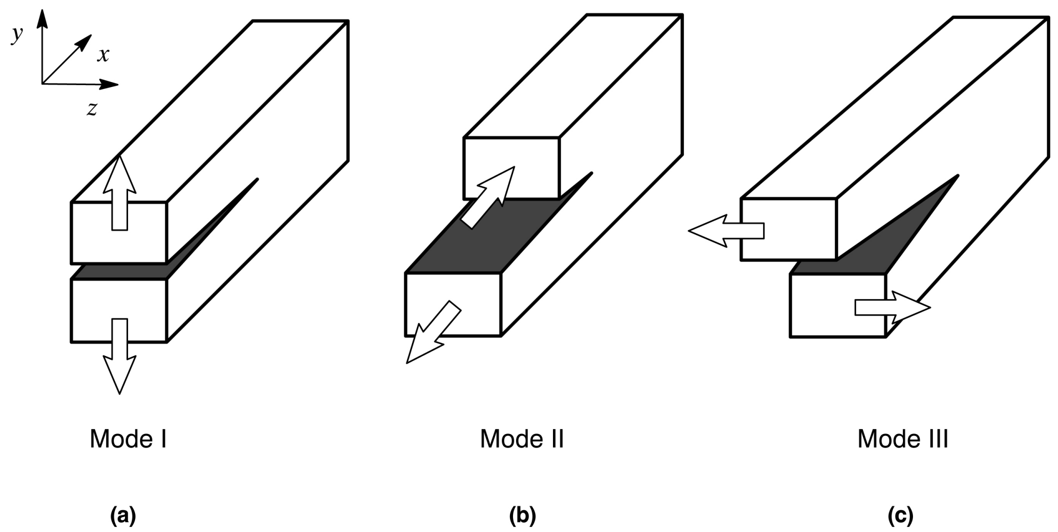

Figure 3.1: *Loading modes acting on a crack: (a) Opening (normal) mode; (b) In-plane shear model and (c) Out-of-plane shear mode.*

3.3 Incorporation of the Threshold Stress

The fundamental expression for the failure probability of a cracked body defined by previous Eq. (3.2) implicitly defines a zero threshold stress for fracture; consequently, stresses vanishingly small compared to the fracture stress 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

$$P_f(J) = 1 - \exp\left\{ -\frac{1}{V_0} \int_\Omega \left[\frac{\sigma_{eq}(J) - \sigma_{th}}{\sigma_u} \right]^m d\Omega \right\} \tag{3.6}$$

where σ_{th} is the threshold stress and has the physical interpretation of a lower bound strength for fracture. Here, the failure probability for the cracked solid is zero for any stress below σ_{th}. When the maximum principal stress criterion is adopted, the above Eq. (3.6) yields

$$P_f(J) = 1 - \exp\left\{ -\frac{1}{V_0} \int_\Omega \left[\frac{\sigma_1(J) - \sigma_{th}}{\sigma_u} \right]^m d\Omega \right\} \quad . \tag{3.7}$$

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. Indeed, as shown by Ruggieri and Dodds [4] and Ruggieri [5], such refinement does not appear to provide significant improvements in predictions of the fracture behavior. Although the debate over a physically meaningful value for has obvious importance, the standard methodology adopted in ***WSTRESS*** utilizes the simplest form of the limiting distribution for the fracture stress by conveniently setting $\sigma_{th} = 0$ in Eqs. (3.6) or (3.7). All subsequent procedures and results are equally valid for any $\sigma_{th} \geq 0$ (which should be adopted or known *a priori*) by simply defining the equivalent stress as $\bar{\sigma}_{eq} = \sigma_{eq} - \sigma_{th}$.

3.4 The Weibull Stress for Growing Cracks

As developed above, 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 the CTOD at onset of crack growth initiation, δ_{Ic}, should not alter the Weibull stress parameters, m and σ_u (which are considered material properties in the present context) and 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 [4].

Figure 3.2 illustrates the development of the active fracture process zone (here defined as the loci where $\sigma_1 \geq \Lambda\sigma_{ys}$, 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 $\sigma_1 \geq \Lambda\sigma_{ys}$ 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

$$\sigma_w = \left[\frac{1}{V_0} \int_{\hat{\Omega}} \sigma_{eq}^m d\hat{\Omega} \right]^{1/m} \tag{3.8}$$

where $\hat{\Omega}$ denotes the active volume of the fracture process zone, $\sigma_1 \geq \Lambda\sigma_{ys}$, which moves forward with the advancing tip. Now, by adopting the maximum principal stress criterion so that the equivalent tensile stress, σ_{eq}, is takes as the maximum principal stress, σ_1, the Weibull stress for a growing crack is then expressed as

$$\sigma_w = \left[\frac{1}{V_0} \int_{\hat{\Omega}} \sigma_1^m d\hat{\Omega} \right]^{1/m} \quad . \tag{3.9}$$

The above generalization of σ_w to include ductile tearing maintains the relative simplicity of the computations while, at the same time, fully incorporating the changes in the stress field ahead of the crack tip due to small amounts of crack growth.

3.5 Effects of Plastic Strain on Cleavage Fracture

The procedures for evaluating σ_w discussed thus far have not explicitly considered the strong effects of near-tip plastic strain on cleavage microcracking which thereby alter the microcrack distribution entering into the local criterion for fracture. Previous fundamental work [49, 50] clearly shows the strong effect of plastic deformation, in the form of inhomogeneous arrays of dislocations, on microcrack nucleation which triggers cleavage fracture at the microlevel of the

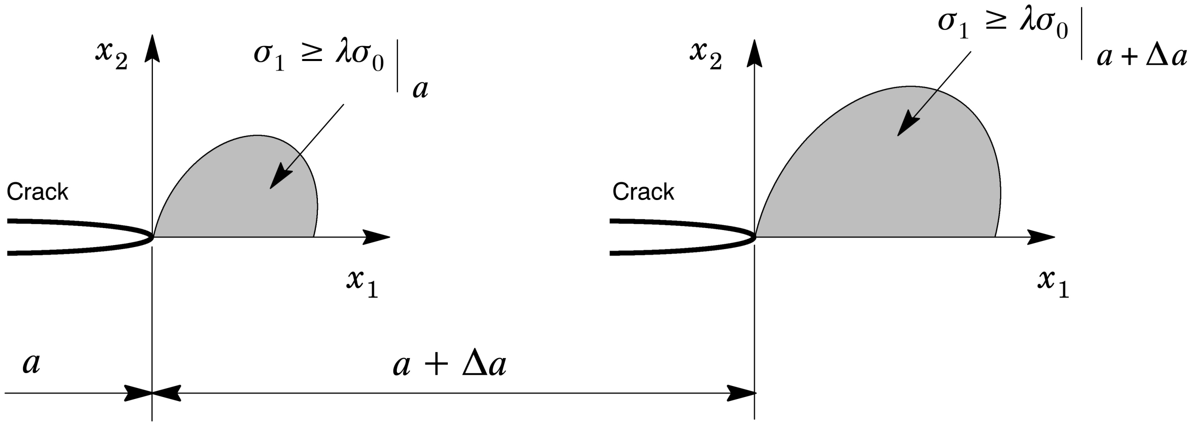

Figure 3.2: *Evolution of the fracture process zone for a growing crack.*

material. This section follows closely the major results of Ruggieri and Dodds (R&D) [6, 7, 66] to introduce a local approach to fracture incorporating the effects of plastic strain on the statistics of microcracks, which have a direct bearing on predictions of specimen geometry effects on cleavage fracture. Primary attention is given to two different functional forms defining the dependence of microcrack propagation on local plastic strain that provide the basis to assess effects of constraint loss and plastic strain on cleavage fracture toughness. Readers are referred to those articles for further details on the methodology.

The problem addressed here consists in developing a convenient probabilistic description of the local fracture process in an arbitrarily stressed body or structural component containing a macroscopic crack in connection with the local plastic strain fields. Consider again a small volume element, δV, ahead of crack and inside the near-tip fracture process zone (FPZ) shown in Fig. 3.3. Further consider that the stress-strain fields acting on δV can be well represented by the principal stress, σ_1, and associated effective plastic strain, ϵ_p. Fundamental understanding of the (transgranular) cleavage fracture process (see, *e.g.* the review article of Hahn [52]) supports the assumption that only microcracks formed from the cracking of brittle particles, such as carbides, in the course of plastic deformation contribute to cleavage fracture. The following assumption may also be brought to bear: the fraction of fractured particles, Ψ_c, which trigger unstable (cleavage) fracture at the microlevel is an increased function of plastic strain (*i.e.*, Ψ_c increases as the matrix plastic strain also increases [52, 67]). This approximation retains strong contact with the Weibull stress concept introduced by Beremin [1, 2] while, at the same time, developing a convenient expression to describe the failure probability of cracked body under arbitrary loading.

Building upon these arguments, R&D [6, 7], introduced a probability distribution for the cleavage fracture stress expressed as a two-parameter Weibull function [26] in the form

$$P_f(\sigma_1,\ \epsilon_p) = 1 - \exp\left[-\frac{1}{V_0}\int_\Omega \Psi_c(\epsilon_p)\cdot\left(\frac{\sigma_1}{\sigma_u}\right)^m d\Omega\right] \tag{3.10}$$

where Ω is the volume of the near-tip FPZ defined by the near-tip region in which $\sigma_1 \geq \psi\sigma_{ys}$, with σ_{ys} denoting the material yield stress and $\psi \approx 2$. In the above, V_0 is a reference volume

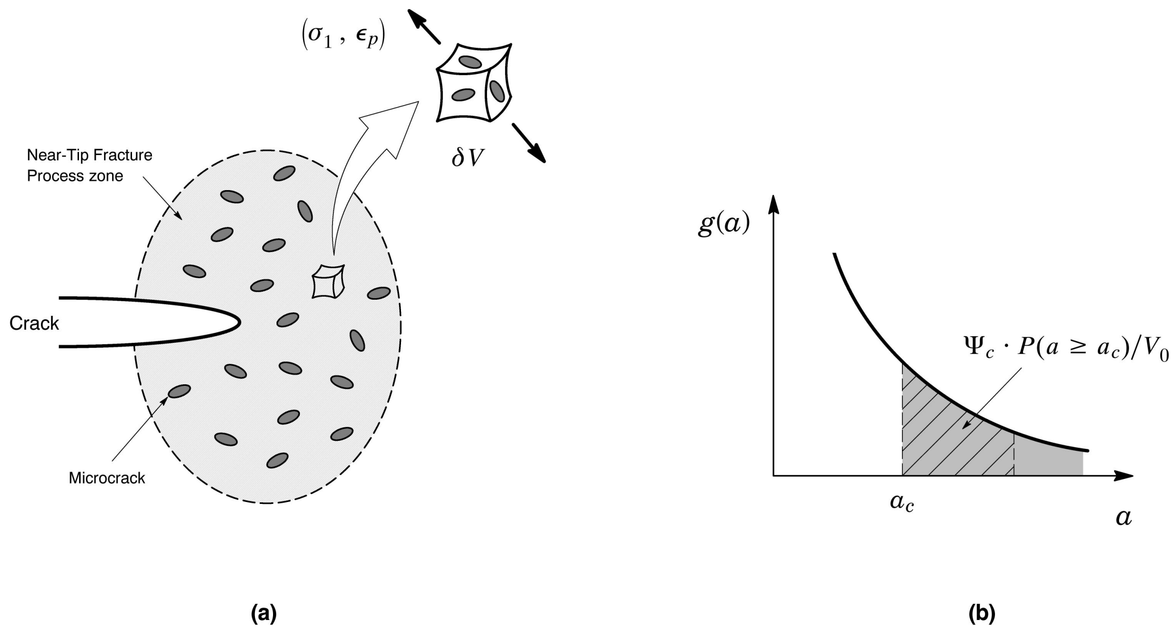

Figure 3.3: *(a) Near-tip fracture process zone ahead a macroscopic crack containing randomly distributed flaws; (b) Schematic of power-law type microcrack size distribution.*

conventionally assigned a unit value, and parameters m and σ_u characterize the Weibull modulus and the scale parameter of the Weibull distribution. A simple manipulation of Eq. (3.10) then yields

$$\tilde{\sigma}_w = \left[\frac{1}{V_0} \int_\Omega \Psi_c(\epsilon_p) \cdot \sigma_1^m d\Omega \right]^{1/m} \quad . \tag{3.11}$$

which is readily associated with a modified form of the Weibull stress, since setting $\Psi_c = 1$ recovers the conventional Beremin model [1, 2].

Previous work of R&D [6] explored different functional forms defining the dependence of microcrack propagation on local plastic strain. The present implementation of ***WSTRESS*** adopts a two-parameter Weibull function to describe the distribution of fracture stress for the particle, σ_{pf}, such that Ψ_c yields [14]

$$\Psi_c = 1 - \exp \left[- \left(\frac{\sigma_{pf}}{\sigma_{prs}} \right)^{\alpha_p} \right] \tag{3.12}$$

where σ_{prs} denotes the reference fracture stress of the particle, α_p is the shape parameter of the Weibull distribution and $\sigma_{pf} = \sqrt{\beta_p \sigma_1 \epsilon_p E_d}$ defines the fracture stress of the particle. Here, σ_1 is the maximum principal stress, ϵ_p is the effective plastic strain for the matrix, E_d is the elastic modulus of the particle and β_p characterizes the particle shape. For typical ferritic materials, α_p and E_d take the values of 4 and 400 GPa as suggested by Wallin and Laukkanen [14]. An elastic modulus of $E_d = 400\,\text{GPa}$ is also within the range of reported values for cementite particles [68, 69]. Moreover, while Wallin and Laukkanen [14] employed a particle shape parameter of 1.3, values of $\beta_p = 1$ can also be used for simplicity since this value only scales σ_{prs} .

Alternatively, following again R&D [6, 7], the fraction of fractured particles can be described by an exponential distribution [26, 60, 70] with parameter λ given by

$$\Psi_c = 1 - \exp(-\lambda \epsilon_p) \tag{3.13}$$

where it is readily understood that the underlying assumption follows a stochastic model in which a Poisson process [60] is adopted to characterize the distribution of fractured particles that trigger cleavage fracture. Within the present probabilistic context, λ thus represents the average rate of Griffith-like microcracks formed from fractured particles with a small strain increment.

A key feature emerging from the previous probabilistic formulations, which is analogous to the Beremin model, is the notion of $\tilde{\sigma}_w$ as a probabilistic crack-tip driving force. Thus, a generalized form of the toughness scaling model (TSM), introduced in early work of Dodds and Anderson [71, 72] and subsequently by Ruggieri and Dodds [4], that include the effects of plastic strain on cleavage fracture, can rationally be extended to correlate fracture toughness behavior in varying crack configurations under different loading and constraint conditions. Section 4.2 briefly describes the toughness scaling methodology employed to calibrate parameter m using two data sets of fracture toughness values.

3.6 Fracture Under Small Scale Yielding Conditions

Consider a case of interest for cleavage fracture assessments in which the crack-tip fields that develop in a fracture specimen or cracked configuration with sufficiently large thickness, B, are well characterized by the small strain HRR fields or, equivalently, by the small scale yielding (SSY) fields [29]. With the equivalent tensile stress, σ_{eq}, defined by the maximum principal stress, σ_1, evaluation of the Weibull stress follows from previous Eq. (3.5) as

$$\sigma_w = \left[\frac{B}{V_0} \int_0^{2\pi} \int_0^{\bar{r}} \sigma_1^m r dr d\theta \right]^{1/m} \quad . \tag{3.14}$$

where r and θ are polar coordinates centered at the crack tip (refer to Fig. 2.2), $\bar{r}$ is the radius of the fracture process zone and B represents the thickness of the component or specimen.

Now define the nondimensional radius, ρ, which is independent of load level (as characterized by J) by $\rho = r/(J/\sigma_{ys})$ such that

$$r = \left(\frac{J}{\sigma_{ys}} \right) \rho \tag{3.15}$$

and

$$dr = \left(\frac{J}{\sigma_{ys}} \right) d\rho \quad . \tag{3.16}$$

Making use of Eqs. (3.15) and (3.16), the Weibull stress, Eq. (3.14) can be rewritten as

$$\sigma_w = \left[\frac{BJ^2}{V_0\sigma_{ys}^2}\int_0^{2\pi}\int_0^{\bar{\rho}}\sigma_1^m \rho d\rho d\theta\right]^{1/m} \tag{3.17}$$

where $\bar{\rho} = \bar{r}/(J/\sigma_{ys})$.

Under SSY conditions, the near-tip principal stress can be expressed in separable form as

$$\sigma_1 = \sigma_{ys} f(\rho,\ n,\ E/\sigma_{ys}) g(n,\ \theta) \tag{3.18}$$

where it is understood the the structure of the principal stress fields is essentially similar to the structure of the HRR fields [29]. Here, f and g are dimensionless functions, E represents the elastic (longitudinal) modulus and n is the strain hardening exponent. Substituting this expression into previous Eq. (3.17), the Weibull stress has the form

$$\sigma_w = \left[J^2\left(\frac{B\sigma_{ys}^{m-2}}{V_0}\right)\int_0^{2\pi}\int_0^{\bar{\rho}}\left[f(\rho,\ n,\ E/\sigma_{ys})g(n,\ \theta)\right]^m \rho d\rho d\theta\right]^{1/m} \tag{3.19}$$

where $\bar{\rho}$ is a function of θ and material flow properties but independent of J. For the analysis pursued here, it is convenient to define $\Phi = \int_0^{2\pi}\int_0^{\bar{\rho}}(f\cdot g)^m \rho d\rho d\theta$ to restate σ_w as

$$\sigma_w = \left[\frac{B\Phi\sigma_0^{m-2}}{V_0}J^2\right]^{1/m} \tag{3.20}$$

which describes the dependence of σ_w on J for any m-value and different material flow properties through the function Φ.

Directing now the attention to the two-parameter Weibull distribution of σ_w and combining Eq. (3.20) with Eq. (3.4), the resulting distribution has the form

$$F(J_c) = 1 - \exp\left[-\left(\frac{J_c}{\beta}\right)^2\right] \tag{3.21}$$

where the scale parameter, β, is then given by

$$\beta = \left(\frac{V_0\sigma_u^m}{B\Phi\sigma_0^{m-2}}\right)^{1/2} \quad . \tag{3.22}$$

The previous analysis clearly demonstrates that, under SSY conditions or, more specifically, under J-controlled conditions, macroscopic values of cleavage fracture toughness are well described by a two-parameter Weibull distribution with a fixed value for the shape parameter defined by $\alpha = 2$. A simple inspection of Eq. (3.21) also reveals a rather strong dependence of the toughness level, as characterized by β, on material flow properties, the function Φ and the Weibull stress parameters, $(m,\ \sigma_u)$. Similar results paralleling the previous SSY solution have been obtained earlier by Mudry [2] and Minami et al. [18].

3.7 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 employed in the present work. In isoparametric space, the current (deformed) Cartesian coordinates of any point inside a 8-node tri-linear element are related to the parametric coordinates through the relationship [73, 74, 75]

$$x_i = \sum_{k=1}^{8} N_k x_{i,k} \quad , \quad i = 1,\ 2,\ 3 \tag{3.23}$$

where N_k are the shape functions corresponding to node k and $x_{i,k}$ are the current (deformed) nodal coordinates, $x_{i,k} = X_{i,k} + u_{i,k}$, where $X_{i,k}$ represent the undeformed (initial) nodal coordinates and $u_{i,k}$ denote the nodal displacements. The shape functions have standard form

$$N_k = \frac{1}{8} \prod_{i=1}^{3} (1 + \eta_i \eta_{i,k}) \quad , \quad k = 1, \ldots, 8 \tag{3.24}$$

where $\eta_{i,k}$ denotes the isoparametric coordinates of node k.

Let $\mid J_{xyz} \mid$ denote the determinant of the standard coordinate Jacobian transformation between deformed Cartesian and parametric coordinates. Then using standard procedures for integration over element volumes, the Weibull stress defined by previous Eq. (3.5) has the form

$$\sigma_w = \left[\frac{1}{V_0} \sum_{n_e} \int_{-1}^{+1} \int_{-1}^{+1} \int_{-1}^{+1} \sigma_1^m \mid J_{xyz} \mid d\eta_1 d\eta_2 d\eta_3 \right]^{1/m} \tag{3.25}$$

which represents the integral form in isoparametric space of Beremin's formulation [1]. In the above, n_e is the number of elements inside the fracture process zone near the crack tip and the Jacobian matrix, J_{xyz}, is given by

$$J_{xyz} = \begin{bmatrix} \dfrac{\delta x_1}{\delta \eta_1} & \dfrac{\delta x_1}{\delta \eta_2} & \dfrac{\delta x_1}{\delta \eta_3} \\ \dfrac{\delta x_2}{\delta \eta_1} & \dfrac{\delta x_2}{\delta \eta_2} & \dfrac{\delta x_2}{\delta \eta_3} \\ \dfrac{\delta x_3}{\delta \eta_1} & \dfrac{\delta x_3}{\delta \eta_2} & \dfrac{\delta x_3}{\delta \eta_3} \end{bmatrix} \quad . \tag{3.26}$$

Again, the process zone used here includes all material inside the loci, $\sigma_1 \geq \Lambda \sigma_{ys}$, with $\Lambda \approx 2$. For computational simplicity, an element is included in the fracture process zone if the principal stress, σ_1, computed at the centroid of the element, $\eta_1 = \eta_2 = \eta_3 = 0$, exceeds $\Lambda \sigma_{ys}$.

4

Calibration of Weibull Stress Parameters

This section describes the theoretical basis and numerical implementation of the procedure for estimation of the Weibull parameters (m, σ_u) appearing in Eq. (3.4). Specifically, the calibration scheme focuses on determining the Weibull modulus m; the scale parameter, σ_u, is easily determined after parameter m is calibrated. For analyses employing a threshold stress, $\sigma_{th} \geq 0$, and the limiting distribution for the fracture stress in the form of Eqs. (3.6) or (3.7), the procedures described in this section are equally valid; defining a new random variable $\bar{\sigma} = \sigma_1 - \sigma_{th}$ (or $\bar{\sigma} = \sigma_{eq} - \sigma_{th}$) still preserves the functional form of the Weibull stress given by Eq. (3.3) or (3.5).

4.1 Limitations of Current Calibration Procedures

Previously developed procedures to calibrate parameters (m, σ_u) (see [1, 4, 18, 22] for additional details) employ measured toughness data for cleavage fracture (such as J_c-values) to define corresponding values of the Weibull stress at fracture, denoted $\sigma_{w,c}$; these values form the basis to estimate the Weibull parameters for the material without making recourse to detailed metallographic measurements. The methodology builds upon an iterative procedure incorporating a finite element description of the crack-tip stress fields and measured values of fracture toughness.

This calibration procedure [1, 4, 18, 22] seeks to determine parameters (m, σ_u) of the probability distribution given by Eq. (3.4) that satisfies the identity $F(J_c) = F(\sigma_{w,c})$, where $F(J_c)$ is the probability distribution for fracture toughness given by Eq. (2.2) and $F(\sigma_{w,c})$ is the probability distribution for the Weibull stress given by Eq. (3.4). Now, let $F_{FEM}(\sigma_w)$ and $F_{exp}(\sigma_w)$ denote the distributions of σ_w corresponding to the stress state obtained through a finite element analysis and the one obtained through fracture toughness testing, respectively. By postulating that $F_{FEM}(\sigma_w)$ and $F_{exp}(\sigma_w)$ have identical distributions, the calibration process becomes one of determining a set of parameters ($\hat{m}$, $\hat{\sigma}_u$) which satisfies this condition. The algorithm starts by determining $\sigma_{w,FEM} = h(J,\, m)$ for an initial estimate of m, denoted m_0, where $h(J,\, m)$ denotes the computed functional relationship between J in the finite element model and the Weibull stress for the specified value of m. The experimental Weibull stress, $\sigma_{w,exp}$, corresponding to each experimental toughness value is found by substituting J_c into $h(J,\, m)$. By applying a standard statistical analysis (such as the maximum likelihood method [26]) to these $\sigma_{w,exp}$-values, the estimates of the Weibull stress parameter, $(\hat{m}_1,\ \hat{\sigma}_{u,1})$ are found for the distribution $F_{exp}(\sigma_w)$. If $m_0 \neq \hat{m}_1$, the process starts anew with the distribution $F_{FEM}(\sigma_w)$ computed for $m = \hat{m}$.

A fundamental assumption underlying the above calibration procedure is that each toughness value, J_c, of the data set defines a corresponding $\sigma_{w,c}$-value for a fixed m as illustrated in Fig. 4.1. Consequently, the associated identity $F(J_c) = F(\sigma_{w,c})$ coupled with Eq. (2.2) and Eq. (3.4) permits generalizing a relationship between J and σ_w in the form

$$\left(\frac{\sigma_w}{\sigma_u}\right)^m = \left(\frac{J}{J_0}\right)^\alpha \quad . \tag{4.1}$$

which yields

$$\sigma_w = C_m J^{\alpha/m} \tag{4.2}$$

with $C_m = \sigma_u^m / J_0^\alpha$.

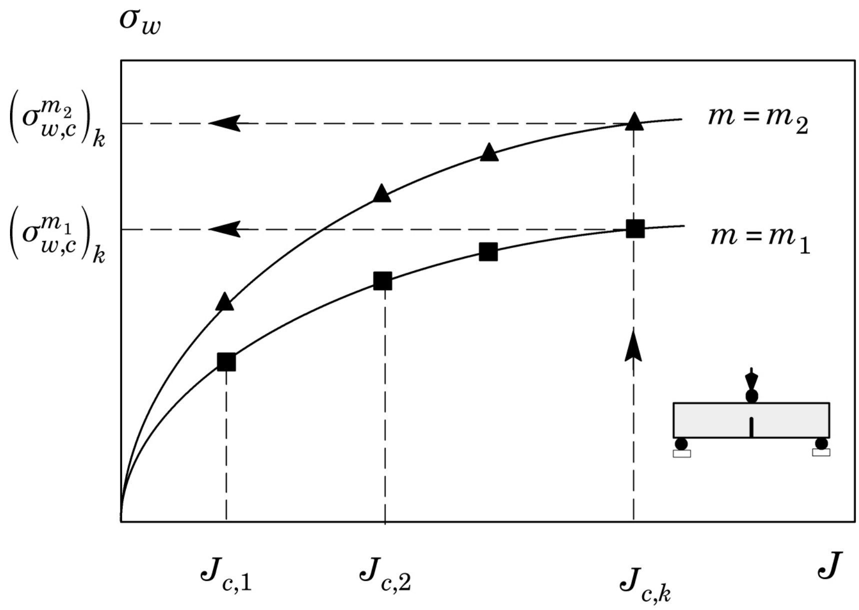

Figure 4.1: *Schematic* σ_w vs. J *trajectories for two arbitrary* m*-values.*

However, a major point of criticism of the calibration process described above is that the identity $F(J_c) = F(\sigma_{w,c})$ and the above Eq. (4.1) are always satisfied for any value of parameter m. Consider the data set for toughness values, $J_{c,k}$, shown as solid symbols in Fig. 4.1 and its equivalent data set of σ_w for two *arbitrary* m-values, $m = m_1$ and $m = m_2$. Now, consider the two-parameter Weibull distribution given by Eq. (2.2) which describes the J_c-values with fixed parameters $(\alpha,\ J_0)$. Each $J_{c,k}$-value uniquely defines a failure probability for the cracked configuration, denoted $F(J_{c,k})$. Let again $h(J,\ m)$ denote the computed functional relationship between J in the finite element model and the Weibull stress for a specified value of m. Because each $J_{c,k}$-value is transformed into corresponding Weibull stress values, $\left(\sigma_{w,c}^{m_1}\right)_k$ or $\left(\sigma_{w,c}^{m_2}\right)_k$, through $h(J,\ m)$, it becomes clear that $F(J_c) = F\left[\left(\sigma_{w,c}^{m_1}\right)_k\right] = F\left[\left(\sigma_{w,c}^{m_2}\right)_k\right]$. Here, there exists no strict requirements to assume SSY or LSY conditions as long as Eq. (4.1) remains valid. In other words, because $F(J_c)$ and $F(\sigma_{w,c})$ are coupled distributions, the non-uniqueness of parameter m holds true as long as there exists a Weibull distribution describing the measured toughness values *and* the associated Weibull distribution for σ_w (see Fig. 4.1). The issue of non-uniqueness of the Weibull modulus, m, is also convincingly demonstrated by Gao et al. [24] and Ruggieri et al. [23]; in their work, numerical arguments provide support for the non-uniqueness of parameter m under SSY conditions. Consequently, it is not possible to calibrate parameters (m, σ_u) using the procedure previously outlined. Further examination reveals that this iteration scheme to determine parameter m merely reflects, at best, the errors in crack-tip fields that emerge in numerical analyses of fracture specimens due to meshing refinement, element behavior, integration schemes, etc.

4.2 Toughness Scaling Methodology Using Weibull Stress Trajectories

Ruggieri and Dodds [4, 21, 44] proposed a toughness scaling model based upon the Weibull stress concept to assess the effects of constraint variations on cleavage fracture toughness data. Here, the central feature lies in the interpretation of σ_w as the (probabilistic) *crack tip driving force* coupled with the simple axiom that cleavage fracture occurs when σ_w reaches a critical value, $\sigma_{w,c}$. For the same material at a fixed temperature, the scaling model requires the attainment of a specified value for σ_w to trigger cleavage fracture across different crack configurations even though the loading parameter (measured by the J-integral in the present context) may vary widely due to constraint loss. In the probabilistic context adopted here, attainment of equivalent values of Weibull stress in different cracked configurations implies the same *probability* of cleavage fracture.

Figure 4.2(a) illustrates the procedure to assess the effects of constraint loss on cleavage fracture behavior needed to scale toughness values for different cracked configurations. The procedure employs J as the measure of macroscopic loading, but remains valid for other measures of remote loading, such as K_J or CTOD (δ). Without loss of generality, Fig. 4.2(a) displays curves of σ_w *vs.* J for a high constrained configuration (such as a deep notch SE(B) specimen), denoted as configuration **A**, and a low constraint configuration (such as surface crack specimen under tension loading), denoted as configuration **B**. Very detailed, nonlinear 3-D finite element analyses provide the functional relationship between the Weibull stress (σ_w) and applied loading (J) for a specified value of the Weibull modulus, m. Given the toughness value for the high constraint fracture specimen, denoted as J_c^A, the lines shown on Fig. 4.2(a) readily illustrate the technique used to determine the corresponding toughness value for the low constraint configuration, denoted as J_c^B.

To facilitate interpretation of the parameter calibration for the tested steel presented in Chapter 7, it is useful to recast the scale model into constraint correction curves as shown on Fig. 4.2(b). This plot provides pairs of normalized J_c-values, represented by (J_c^A, J_c^B), that produce the same $\sigma_{w,c}$ (and thus the same failure probability). Reference lines are shown which define a constant ratio of *constraint loss*, *e.g.*, $J_c^B = 1.2\, J_c^A$ which implies that the average J_c-value for configuration

B must be 20% larger than the J_c-value for configuration **A** to generate the same σ_w-value. For each Weibull modulus, m, the constraint correction curves agree very well early in the loading history while configuration **B** still maintains high levels of stress triaxiality across the crack front. Once loss of crack-tip constraint occurs, the curves for the low constraint configuration deviate significantly from high constraint conditions. The Weibull modulus, m, does have an appreciable effect on predictions of constraint loss; increased m values for the present example indicate a higher load level at the onset of constraint loss and a reduced rate of constraint loss under further loading.

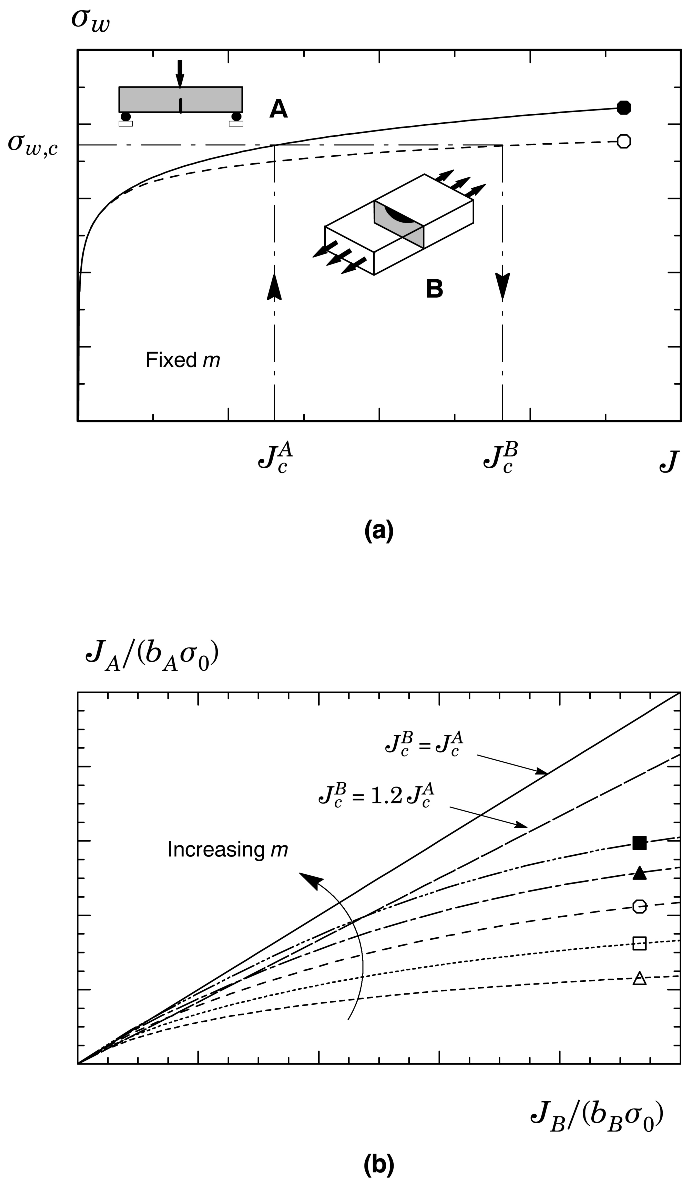

Figure 4.2: *(a) Scaling procedure based on the Weibull stress concept to correct toughness values for different crack configurations; (b) Constraint corrections curves derived from the toughness scaling model in which the J-values are normalized by the remaining crack ligament and a reference stress, σ_0, representing the material yield stress.*

4.3 Parameter Calibration Using Weibull Stress Trajectories

The previous section exhibits the essential features of Weibull stress based constraint corrections for crack configurations (specimen geometries) with different levels of stress triaxiality. The present implementation of ***WSTRESS*** adopts a parameter calibration scheme that uses the scaling methodology previously outlined to correct measured toughness distributions for different crack configurations. The procedure extends previous work by Gao et al. [24] and Ruggieri et al. [23] to calibrate parameters (m, σ_u) using high constraint (SSY) and low constraint (LSY) fracture toughness data measured at the same temperature and loading rate. Because each measured J_c^B-value is corrected to its equivalent J_c^A-value, the statistical (Weibull) distribution of J_c^B-values is also corrected to an equivalent statistical (Weibull) distribution of J_c^A-values. Consequently, the present scheme simply defines the calibrated value of parameter m for the material under consideration as the value that corrects the characteristic toughness J_0^B (*i.e.*, the scale parameter of Eq. (2.2) - see Section 2.2) to its equivalent J_0^A. Because parameter m is assumed independent of specimen geometry (as long as the framework upon which the Weibull stress is based remains valid), the scheme remains equally applicable when two sets of fracture toughness data from different crack configurations, but with sufficient differences in the evolution of σ_w *vs.* J, are used (e.g., 1T SE(B) specimens with $a/W = 0.5$ and $a/W = 0.2$).

The following steps describe the key procedures in the calibration scheme implemented in ***WSTRESS***. Chapter 7 illustrates application of the process for a low alloy, structural steel.

Step 1

Test two sets of specimens with different crack configurations (**A** and **B**) in the DBT region to generate two distributions of fracture toughness data. Select the specimen geometries and the common test temperature to insure different evolutions of constraint levels for the two configurations. No ductile tearing should develop prior to cleavage fracture in either sets of tests. Several alternatives to obtain the two sets of toughness values at the same test temperature include: 1) Test high constraint deep-notch SE(B)s or C(T)s as configuration **A**. To insure SSY conditions at fracture, set the specimen size so that $J_c \leq (b\sigma_{ys}/M)$ for each specimen, with M conservatively set to $60 \sim 100$ [76]. For configuration **B**, use similar size SE(B) specimens but with shallow-notches, *i.e.*, $a/W = 0.2$. These will undergo significant constraint loss when the deep-notch values just satisfy the suggested deformation limit; 2) Test large (**A**) and small (**B**) deep-notch SE(B) specimens having the same $a/W \geq 0.5$ ratio. Set the large specimen size to provide high constraint conditions. Set the small specimen size to insure sufficient loss of constraint at fracture for most specimens.

Step 2

Perform detailed, 3-D finite element analyses for the tested specimen geometries. The mesh refinements must be sufficient to insure converged σ_w *vs.* J histories for the expected range of m-values and loading levels. When using fracture specimens with similar overall geometry but different in-plane constraint (e.g., 1T SE(B) specimens with $a/W = 0.5$ and $a/W = 0.2$), plane-strain analyses may also provide satisfactory results.

Step 3

Assume an m-value. Compute the σ_w *vs.* J history for configurations **A** and **B** to construct the toughness scaling model relative to both configurations.

Step 4

Constraint correct J_0^B to its equivalent J_0^A (*i.e.*, the corrected value of the scale parameter for the assumed m-value). Define the error or *residual* of toughness scaling as $R(m) = (J_{0,m}^A - J_0^A)/J_0^A$. If $R(m) \neq 0$, repeat ***Step 3*** for additional m-values.

Step 5

Plot $R(m)$ *vs.* m as illustrated in Fig. 4.3. The calibrated Weibull modulus makes $R(m) = 0$ within a small tolerance.

Step 6

Compute the σ_u-value. After m is determined, σ_u is obtained easily from the σ_w *vs.* J history for the calibrated m-value. σ_u equals the Weibull stress value at $J = J_0^A$ or $J = J_0^B$ in the corresponding configuration.

4.4 Minimization of the Residual Function

A key step in the calibration procedure implemented in ***WSTRESS*** is the minimization of the error function $R(m) = (J_{0,m}^A - J_0^A)/J_0^A$ described above. The funcion $R(m)$ defines the *residual* of the constraint correction for the toughness values, $J_0^B \rightarrow J_0^A$, for a given m-value. Figure 4.3 illustrates the variation of $R(m)$ with parameter m for a given material. The calibrated Weibull modulus corresponds to the minimum of $R(m)$.

To determine the minimum of the function $R(m)$, ***WSTRESS*** implements an optimal method of function minimization based on a golden section search algorithm [77]. The method searches for the minimum of a function by successive bracketing a triplet of points; the routine then performs a golden section search for the minimum. The algorithm is linearly convergent and yields very robust minimum values provided a good initial triplet of points is chosen. Readers are referred to reference [77] for further details.

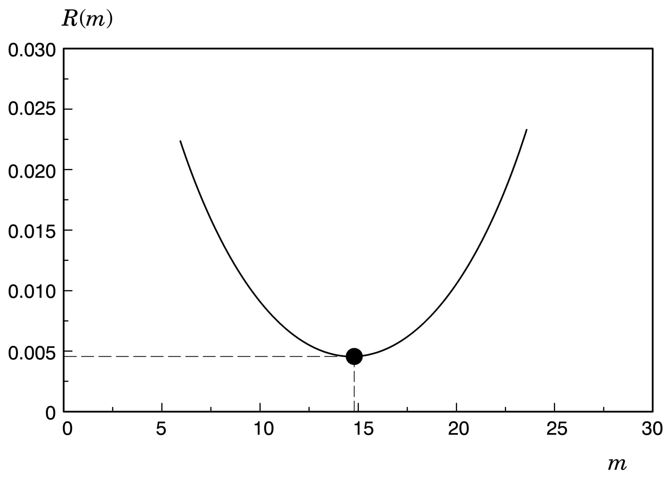

Figure 4.3: *Schematic variation of the residual function, $R(m)$, with parameter m.*

5

Syntax of Commands and Input Parameters

5.1 Using *WSTRESS*

WSTRESS takes input commands in a free-form command language from a file to define the model, material properties, solution parameters and experimental data. Input files may include extensive user comments and are, thus, generally self-documenting. Input finite element results consist of files stored in Patran binary or ASCII format associated with WARP3D [27] finite lement code. Future versions of ***WSTRESS*** will have the capability of handling finite element results from ABAQUS [28] finite element code.

The current version of ***WSTRESS*** executes in foreground mode in DOS environment using the shell command

```
wstress < input_file > output_file
```

or

```
wstress < input_file
```

where the last command simply displays the results to the standard output device defined by the screen Windows command line (DOS shell).

5.2 Syntax Conventions

The input translators for ***WSTRESS*** provide a problem oriented language (POL) command structure to simplify specification of model and solution parameters. This section describes the conventions and notation employed throughout the manual to explain commands.

Input to ***WSTRESS*** appears as a sequence of English-like commands in the form

`maximum iterations` < 100 >

where the words `maximum` and `iterations` form a command which is followed by a descriptor (in the above example an integer number).

The appearance within a ***WSTRESS*** command of a descriptor of the form

< `integer` >

or

< `real` >

implies that the user should enter an item of data within that position in the statement of the class described by the descriptor, such as an *integer* or *real* in the above examples. The command

`maximum iterations` < `integer` >

implies that the word *iterations* is to be followed by an integer, such as 30 or 100.

5.2.1 Descriptors

The following are definitions of most of the descriptors used within the language. Those not described below are explained when they first occur in the text.

< `integer` >

a series of digits of integer character optionally preceded by a plus or minus sign. Examples are 121, +300, -410.

< `real` >

a series of digits with a decimal point included, or series of digits with a decimal point followed by an exponential indicating a power of 10. Real numbers may be optionally signed. Examples are 1.0, -2.5, 4.3e-01.

< `number` >

is either a < `real` > or an < `integer` >. The input translator performs mode conversion as needed for internal storage.

< `label` >

is a series of letters and digits. The sequence must begin with a letter. Input translators also accept the character underbar (or underscore), _, as a valid letter. Labels may have the form `bend_bar`, for example, to give the appearance of multiple words for readability.

< `string` >

is any textual information enclosed in apostrophes (') or quotes ("). An example is "this is a string".

< `list` >

is the notation used to indicate a sequence of positive integer values - usually node and element numbers. Lists generally contain two forms of data that may be intermixed with the same list. The first form of data is a series of integers optionally separated by commas. An example is 1, 3, 6, 10, 12. The second common form of a list implies a consecutive sequence of integers and consists of two integers separated by a hyphen. An example is 1-10, which implies all integers in the sequence 1 through 10. An extension of this form implies a constant increment, e.g., 1-10 by 2 implies 1, 3, 5, 7, 9. A third form defined by the key word `all` is sometimes permitted, and implies all physically meaningful integers. The forms of lists are often combined as in ... nodes 1-100 by 3, 200-300, 500-300 by - 3. In some specific cases, such as when inputing experimental fracture touhness values, the `list` descriptor also allows the input of a sequence of real number (either negative or positive).

5.2.2 Command Structure

In many instances, more than one word is acceptable in a given position within a command. The choices are listed one above the other in the command definition. The command definition

$$\texttt{active process zone} \left\{ \begin{array}{c} \texttt{mises stress} \\ \texttt{principal stress} \end{array} \right\}$$

indicates that each of the following commands are acceptable

`active process zone mises stress`

`active process zone principal stress`

Optional words and phrases are enclosed with parentheses, ( ), like in the command

`format (of) fe – results patran type binary`

In order to be more descriptive within the command definitions, actual data items (those denoted with < > in the definition) are sometimes described in terms of their physical meaning and followed by the type or class of data item which can be used in the command. For example the command,

`structure < name of structure : label >`

implies that the data item following the word `structure` is the name of the structure and must be a descriptor of type < `label` >. Examples of acceptable commands are

`structure bend_bar`

or

`structure seb`

while

`structure 1tseb`

is not acceptable since the name of the structure is not a label (*labels must begin with a letter*)

5.2.3 Other Syntaxes

The following are definitions of other syntaxes used within the language.

Continuation lines
A comma (,) placed at the end of a line causes the subsequent data line to be considered a logical continuation of the current line. There is no limit on the number of continuation lines. Continuation can be invoked at any point in any command.

Comment lines

Comments may be placed in the input following a Fortran style. The letter `c` or `C` appearing in physical column 1 of the data line marks it as a comment line. The line is read and (possibly) echoed by the input translator. The content is ignored and the next data line read.

Comments within lines

Comments may also be placed just after a given syntax of commands within the line following a ! character. The line is read and (possibly) echoed by the input translator and the remaing text following the ! is interpreted as a comment.

Line termination

Line termination is accomplished in one of three ways. First, the last column examined by the input translators is column 72. Secondly, after encountering the first data item on a card, the translators count blanks between data items. If 40 successive blanks are found, the remainder of the line is assumed blank. Finally, a $ indicates an end of line. Space following the $ is ignored by the input translators and is often used for short comments.

5.3 Analysis Type Definition

While ***WSTRESS*** has been primarily designed to perform the calibration of the Weibull stress parameters (m, σ_u) based on the toughness scaling methodology (TSM) introduced by Ruggieri and Dodds [4], future versions of the code will also include other capabilities to support some key applications related to the probabilistic framework for cleavage fracture addressed in the present work. In particular, evaluation of the cleavage failure probability based on the measured distribution of carbides and the associated Griffith-like microcracks is of great interest as a means to mitigate the calibration issues that often arises from applications of the conventional Weibull stress model.

To drive the correct execution of the code, a specific analysis type must be assigned to ***WSTRESS*** before any other command in the input file. The first command line of the input file defines the analysis type in the form

`wstress analysis type` $<$ `analysis type : label` $>$

The current version of ***WSTRESS*** implements the basic type of analysis defined by calibration of the Weibull stress parameters using two sets of fracture toughness data. This analysis type and related commands in connection with the parameter definitions are defined next in Chapter 6.

6

Calibration of Weibull Stress Parameters

6.1 Analysis Type

Calibration of the Weibull stress parameters using two sets of fracture toughness data is invoked in WSTRESS using the command

```
wstress analysis type   parameter calibration
```

The above command line must be the first command interpreted by the input processor. This command is followed by a series of statements to define the analysis parameters which are specific to the parameter calibration routines implemented in ***WSTRESS***.

6.2 Blocks of Subcommands

Following the definition of the analysis type described above, the input file syntax is composed by blocks of subcommands, which must necessarily be specified (otherwise a syntax error will occur), followed by the keyword `end`. The measured values of fracture toughness for the specimen or structure under analysis described in the block `experimental data` may also be defined by the parameters of the corresponding Weibull distribution. Scanning of input parameters stops when the keyword `end` is found by the translator. Each block is delimited by the braces { and } as in the following example:

```
wstress analysis type parameter calibration
c
material properties
c
  material a515 {
```

```
    yield stress 320
    young modulus 205000
    poisson ratio 0.3 }
c
crack configuration sebaw5
c
  model definition {
    symmetry factor 4
    get files from directory sebaw5
    input mesh from file sebaw5_coor
    assign elements 1 - 27368 material a515
    input loading parameter from packet file sebaw5_jval
    format fe - results patran type ascii }
c
  experimental data {
    79.6   21.7   47.1   25.3   65.4   17.5   66.2   63.8   69.0 }
c
crack configuration sebaw2
c
  model definition {
    symmetry factor 4
    get files from directory sebaw2
    input mesh from file sebaw2_coor
    assign elements 1 - 25688 material a515
    input loading parameter from packet file sebaw2_jval
    format fe - results patran type ascii }
c
  experimental data {
    23.8   44.3   44.8   59.5   88.6   91.4   101.2   101.2   101.9 141.0 184.2 }
c
analysis parameters
c
  fracture process zone {
    active process zone principal stress
```

```
    fracture criterion principal stress
    process zone size parameter 2.0 }
c
  solution parameters {
    warp3d release V18
    parameter calibration on
    loading parameter j - integral domain 30
    compute steps for structure sebaw5 20 - 480 by 20
    compute steps for structure sebaw2 20 - 600 by 20
    convergence tolerance 0.01
    maximum iteration 100
    plastic strain effect off }
c
  statistical parameters {
    initial shape parameter 20
    reference volume 1.0
    threshold stress 0
    estimation method mlh }
```

6.3 Material Properties

This command manipulates the input of material properties used in the calibration analyses and in the experimental testing program. As presently implemented only one set of material properties can be defined. The current version of ***WSTRESS*** does not have the capability of computing the Weibull stress for multilayered solids, such as a crack located on the boundary between the weld metal and the base material in weldments.

6.3.1 Material Identification

The material under analysis must have a unique identification (label or name) to be used all over the computations. The syntax for assigning a name to a material employed in the analysis is as follows:

```
material < material identification : label >
```

6.3.2 Material Property Specifications

A specific set of mechanical properties must be assigned to the material employed in the analysis. Currently, only the yield point or yield stress, σ_{ys}, is used as the mechanical property for the computations. *This mechanical property must be the same as the one used in the finite element analyses.* While the Young's modulus, E, and the Poisson's ratio, ν, are not used in the computation of the present form of the Weibull stress, users are encouraged to input these values for documentation purposes. The commands to specify the material properties are:

```
yield stress < number >

young modulus < number >

poisson ratio < number >
```

6.4 Crack Configuration

This block of commands defines specific information associated with the models for the specimens (crack configurations) employed in the testing program and the experimental toughness data associated with each tested specimen. Since the calibration procedure for parameter m implemented in the current version of ***WSTRESS*** is based upon fracture toughness data measured from two sets of specimens (denoted **A** and **B** - see Chapter 4), each crack configuration must be specified by a `crack configuration` command as follows

```
c
crack configuration < structure identification : label >
c
```

6.4.1 Model Definition

The `model definition` section defines the finite element model, specific information associated with the meshing and the format for finite element result files. A typical block consists of the following subcommands.

6.4.1.1 Model Symmetry

Many structures and associated finite element models have planes of symmetry with respect to loading and geometry. Symmetry properties, if used for generation of the finite element results, must be taken into account for computation of the Weibull stress. ***WSTRESS*** uses a *scale* or *multiplication factor* to correctly compute σ_w as needed based upon the number of symmetry planes in the model. The symetry factor enters into the computation of σ_w (or, equivalently, $\tilde{\sigma}_w$) only as a multiplier of the stress integral given by previous Eq. (3.3) or Eq. (3.11) and, therefore, has no effect on the Weibull modulus, m. For example, if geometrical and loading conditions permit modeling of only one quarter of an SE(B) specimen, then the symmetry factor is 4. The command is simply

$$\texttt{symmetry factor} < \texttt{integer} >$$

6.4.1.2 Format for Finite Element Results Files

This command defines the source from which ***WSTRESS*** will obtain the finite element results for the Weibull stress computations. Since the formulations previously derived implicitly employ the Cauchy stresses at the center of element, the numerical results consist essentially of element stresses, element strains and nodal displacements; the present version of ***WSTRESS*** provides no facilities for accommodating nodal stresses and strains. As currently implemented, only results files in standard Patran ASCII or binary format can be taken as input data. The command syntax is:

$$\texttt{format (of) fe} - \texttt{results patran type} \begin{cases} \texttt{ascii} \\ \texttt{binary} \end{cases}$$

WSTRESS defaults to the naming convention of Patran results files adopted in WARP3D FE code [27]. Patran binary files of nodal displacement results and element stress and strain results are termed according to the release of the FE code WARP3D [27]. For versions 17.x (and earlier), the file name convenion is *wnbdxxxxx*, *websxxxxx* and *webexxxx*, respectively, where "*xxxxx*" represents the 5-digit load step number. Similarly, Patran ASCII files of nodal displacement results and element stress and strain results are termed *wnfdxxxxx*, *wefsxxxxx* and *wefexxxx*, respectively. For recent, updated versions from V18.x, the file name convenion is *wnbdxxxxxxx*, *websxxxxxxx* and *webexxxxxxx*, respectively, where "*xxxxxxx*" represents the 7-digit load step number. Likewise, Patran ASCII files of nodal displacement results and element stress and strain results are termed *wnfdxxxxxxx*, *wefsxxxxxxx* and *wefexxxxxx*, respectively. The default format for finite element result files follows the file name convention for V18.x.

6.4.1.3 Input File Directory

To facilitate manipulation of the input files and to avoid having these files in the same directory, users should specify the directory where the input files for each crack configuration are located through the command:

`get files from directory` < `directory name : label` >

6.4.1.4 Nodal Coordinates and Element Incidences

Element incidences (connectivities) and nodal coordinates referenced to the undeformed configuration are required for computation of the Weibull stress. Moreover, the model size (number of nodes and elements) is specified in the input mesh file. In general, it is simpler to edit the original input file used for the finite element analysis in a format compatible with the translator of ***WSTRESS*** as shown in Fig 6.1. The command syntax is:

`input mesh (from) file` < `file name : label` >

6.4.1.5 Element Type

Currently, only 8-node hexahedron (brick) elements with standard quadrature (2x2x2) are supported. Future versions of ***WSTRESS*** will support other element types such as the 20-node brick element. The command syntax is given by:

`element type l3disop order 2x2x2`

Since this option is the *default* setting in ***WSTRESS***, users may omit this command from the `model definition` section.

```
1260  575                                     Mesh information

  1 -.145000000E+02  .700000000E+02  .250000000E+00
  2 -.145000000E+02  .700000000E+02  .000000000E+00
  3 -.108750000E+02  .700000000E+02  .250000000E+00
    :          :                 :                 :       Nodal
    :          :                 :                 :       Coordinates
    :          :                 :                 :
1257 -.440890379E-01  .829215795E-01  .250000000E+00
1258 -.292893108E-01  .707106888E-01  .250000000E+00
1259 -.292893108E-01  .707106888E-01  .000000000E+00
1260 -.440890379E-01  .829215795E-01  .000000000E+00
  1  173  174  146  145  175  176  148  147
  2  175  176  148  147  177  178  150  149
  3  177  178  150  149  179  180  152  151
    :          :          :          :          :          Element
    :          :          :          :          :          Incidences
    :          :          :          :          :
 573  929  930  928  927  897  898  896  895
 574  963  964  962  961  931  932  930  929
 575  931  932  930  929  899  900  898  897
```

Figure 6.1: *Input file for nodal coordinates and element incidences.*

6.4.1.6 Assigning Material Properties to Elements

Assignment of material properties to a given block of elements is accomplished by writing the following command:

`assign elements` $<$ `elem. list :  integer` $>$ (`to`) `material` $<$ `mat. id :  label` $>$

where $<$ `element list` $>$ *must* correspond to the same number of elements specified in the finite element model. Since this release of ***WSTRESS*** does not have the capability of computing the Weibull stress for multilayered solids, such as a crack located on the boundary between the weld metal and the base material in weldments, the *default* value for the element list is `all`; in such case, users may omit this command from the `model definition` section.

6.4.1.7 Loading Parameter Results

The computed J-values at specified load steps (which must be consistent with the finite element results generated by the FE-analysis) are also input through a result file. The command syntax to provide the file name is:

`input loading parameter from file` $<$ `file name :  label` $>$

in which the format-free input lines are described in Fig 6.2.

Step Number	Loading Parameter
10	0.555
20	1.145
30	2.008
.	.
.	.
.	.

Figure 6.2: *Input file format for loading parameter results (J or CTOD).*

6.4.2 Experimental Toughness Data

The `experimental data` section defines the experimental data relative to the fracture mechanics tests. As previously indicated, the loading parameter employed in the analysis should be of the same type as the experimental data (J_c or δ_c). The translator takes as input data all numerical values inside this block irrespective of their ordering; ***WSTRESS*** automatically sorts the input list of experimental data in ascending order. The command to input the toughness data has the form:

```
experimental data { < data list : number > }
```

The measured distribution of toughness data may be anternatively specified in terms of a standard two-parameter Weibull distribution in which the Weibull parameters (α, β) were previously determined using, for example, the maximum likelihood method (see Appendix A) or are given as user-defined values. In particular, the scale parameter of the Weibull distribution, which is associated with the characteristic toughness values, such as J_0, in the present context, is then used in the toughness scaling model (TSM) to calibrate the Weibull stress parameters. The command to define the Weibull parameters has the form

```
experimental data {
  use toughness data with alpha < number > beta < number > }
```

Most often, since the shape parameter of the Weibull distribution describing cleavage fracture toughness under SSY conditions is assigned a fixed value (α = 2 for J_c-distributions whereas

$\alpha = 4$ for K_{Jc}-distributions), specification of this parameter can be ommitted. Thus, the above command can take the simpler form[1]

`use toughness data with beta` $<$ `number` $>$ }

6.5 Analysis Parameters

This block of commands controls the parameters used in the computation of the Weibull stress and in the calibration process. These parameters, unless explicitly specified, are applicable for both configurations **A** and **B** utilized in the calibration procedure (see Chapter 4).

6.5.1 Fracture Process Zone

The `fracture process zone` section defines the parameters used in the description of the (near-tip) fracture process zone and specific information of the local fracture mechanism and fracture criterion. A typical block consists of the following subcommands.

6.5.1.1 Active Fracture Process Zone Definition

WSTRESS typically defines the active fracture process zone near the crack tip, Ω, as the region including all material points satisfying the condition $\sigma_1 \geq \Lambda\sigma_{ys}$, where σ_{ys} is the yield (reference) stress, σ_1 is the maximum principal stress and Λ defines the spatial extent (size) of the fracture process zone. Previous analyses [4] suggest a value of $\Lambda \approx 2$ for most cases while a value of $\Lambda \approx 1.5$ may be necessary for low constraint configurations and low hardening materials. Users are encouraged to explore an *optimal* value for the parameter Λ defining the spatial extent of the fracture process zone in more specific cases; values of Λ too large may artificially reduce the size of the fracture process zone size and cause adverse effects on the Weibull stress computations and calibration of Weibull parameters. In addition, ***WSTRESS*** has the capability of using the plastically deformed region ahead of crack tip as the fracture process zone, *i. e.*, $\sigma_e \geq \Lambda\sigma_{ys}$, where σ_e is the effective Mises stress; this definition is directly related to the formation of microcracks by localized plastic flow (see Section 3.1). Here, $\Lambda \approx 0.9$ is most often adopted. However, both definitions are nearly equivalent, particularly for large values of m (Weibull modulus), since the contribution of stressed material points located at distances sufficiently large from the crack tip, say $> 10 \times$ CTOD, is very small. The default for the fracture process zone region, Ω, is the *loci* of the principal stress $\sigma_1 \geq \Lambda\sigma_{ys}$. The fracture process zone or, equivalently, the domain of integration (see Eq. (3.3) or Eq. (3.5)), is specified by giving the command

[1] The current implementation of ***WSTRESS*** routines does not handle measured toughness distributions defined in terms of K_{Jc}-values.

$$\texttt{active process zone} \begin{cases} \texttt{principal stress} \\ \texttt{mises stress} \\ \texttt{ctod} \end{cases}$$

Because the stress history of material points included in the near-tip fracture process zone affects directly the evolution of the Weibull stress as deformation (loading) progresses, the following command also provides a more specific definition for the fracture process zone in terms of the *instantaneous* or *cumulative* regions (see Sections 3.1 and 3.4):

$$\texttt{zone type} \begin{cases} \texttt{instantaneous} \\ \texttt{cumulative} \end{cases}$$

The instantaneous fracture process zone is defined as the current *loci* of the principal stress $\sigma_1 \geq \Lambda\sigma_0$ (or, equivalently, as the *loci* of the Mises stress $\sigma_e \geq \Lambda\sigma_0$) for both a stationary or an extending crack. For both cases, this region is defined by a *snapshot* of all material points inside the near-tip fracture process zone; each material point being subjected to a local, current stress. The cumulative fracture process zone defines the envelope of all material points that have been included in the fracture process zone in previous stages of loading; such a definition also applies to both a stationary and a growing crack. For advancing cracks, the cumulative fracture process zone then includes material points that were left behind the crack (plastic wake) after its extension. The default type is `instantaneous` fracture process zone.

When the instantaneous fracture process zone ahead of crack tip is adopted, the Weibull stress given by Eq. (3.3) or Eq. (3.5) is, by default, computed using the current stress state. Alternatively, ***WSTRESS*** incorporates a simplified treatment to include damage of material located within the region where partial unloading occurs into the calculation of σ_w. Following Koers and co-workers [19], the maximum stress that the material point has experienced during the entire loading history (generally the peak stress) replaces the current stress in the expression for the Weibull stress. Ruggieri and Dodds [4] provide a detailed discussion on this procedure and how it affects the Weibull stress values. When used in analyses involving crack growth, this option enables the construction of a cumulative fracture process zone using the envelope of maximum stresses experienced by material along the crack plane during growth. The input command to include the stress history in the analysis is as follows:

$$\texttt{stress history} \begin{cases} \texttt{on} \\ \texttt{off} \end{cases}$$

where the default option is `off`. The stress history option must be active when the cumulative fracture process zone is specified.

Finally, parameter Λ defining the spatial extent (size) of the fracture process zone is specified by giving the command

```
process zone size parameter < number >
```

As currently implemented, the default setting for parameter Λ depends on the specified domain of integration. For domains defined by the principal stress, the default value for Λ is 2.0. For domains defined by the Mises stress, the default value for Λ is 0.9.

6.5.1.2 Fracture Criterion

A fracture criterion must be specified to determine the equivalent (tensile) stress, σ_{eq}, acting on a microcrack included into the process zone. As already introduced earlier, this version of ***WSTRESS*** employs only the maximum principal stress criterion to describe unstable propagation of the microcrack. The command syntax is the simply:

```
fracture criterion principal stress
```

6.5.2 Solution Parameters

The `solution parameters` section defines the parameters used directly in the numerical algorithms and solution procedure implemented in ***WSTRESS***. A typical block consists of the following subcommands.

6.5.2.1 WARP3D Release

Recent releases of WARP3D [27] (Release *18.x* and later) generate the Patran compatible result files with assigned names that begin with four letters (nodal result files begin with the letters *wn* whereas element result files begin with the letters *we*) followed by the *7 digit* load step number. However, older versions of WARP3D (Releases *17.x* and *16.x*) adopted a *5 digit* form to reference the load step number. Since each form of the assigned file name must be manipulated slightly differently by the open file routines in ***WSTRESS***, the WARP3D release used to generate the finite element results needs to be specified by the command

$$\texttt{warp3d release} \begin{cases} \texttt{V18} \\ \texttt{V17} \end{cases}$$

where the default option is `V18` thereby allowing users to simply omit this command when Release 18.x and later are used.

6.5.2.2 Execution of Parameter Calibration

While the blocks of commands associated with this analysis type are primarily designed to perform the calibration of Weibull stress parameters using two sets of fracture toughness data in connection with the toughness scaling methodology described in Section 4.2, users may also desire to prevent execution of the parameter calibration routines while, at the same time, computing the Weibull stress trajectories for both crack configuration immediately just before starting the iteration procedure. This proves convenient, in most cases, to determine the evolution of σ_w(or, equivalently, $\tilde{\sigma}_w$) with the loading parameter (J or CTOD) for a fixed value of the Weibull modulus, m. The default option is `on` whereas the option `off` suppresses the iterative procedure.

$$\texttt{parameter calibration} \begin{cases} \texttt{on} \\ \texttt{off} \end{cases}$$

6.5.2.3 Loading Parameter

In the present work, overall fracture conditions and macroscopic loading in the specimen or structure under analysis are defined in terms of J or CTOD (δ). The loading parameter characterize the crack-tip stress fields; ***WSTRESS*** then constructs the evolution of the Weibull stress with J or CTOD (δ). When the iterative procedure is invoked, the loading parameter should be of the same type as the experimental data (J_c or δ_c). The command to define the loading parameter has the form:

$$\texttt{loading parameter} \left\{ \begin{matrix} j - integral \\ ctod \end{matrix} \right\} \texttt{domain} < \texttt{integer} >$$

where the domain number corresponds to the domain (or ring) at the crack front position from which WARP3D [27] evaluates the J-integral. Once a given domain is specified, WSTRESS then builds an internal file containing a two-column data array containing the load steps (taken from the specified range of load steps over which the computations are performed - see Section 6.5.2.4 next) and the corresponding J-values for subsequent use in the Weibull stress computations. As currently implemented, the specification of domain number from which the J-integral is extracted from the loading parameter files must be the same for both crack configurations.

6.5.2.4 Specification of Load Steps

The range of load steps over which the computations are performed must be consistent with the results available from the finite element analysis (Patran results files). The range of load steps that define the (computed) Weibull stress function must accommodate the range defined by the experimental data set for the two crack configurations (**A** and **B**) employed in the testing program. Users should specify any valid integer between the minimum and the maximum number of load steps available from the finite element analysis. Load steps which contain no yielded elements are automatically skipped. The command syntax is:

`compute` (`load`) `steps` (`for`) `structure` < `struct id` : `label` >< `lstep list` : `integer` >

which should be repeated for each crack configurations (**A** and **B**) employed in the testing program (see above example of a typical input block for the `process zone` section.

6.5.2.5 Convergence Tolerance

Convergence of the iterative procedure is assessed by simply evaluating the residual of the error function $R(m) = (J^A_{0,m} - J^A_0)/J^A_0$ (see Section 4.4) in the form $R(m) \leq \chi$, where χ is the tolerance value. ***WSTRESS*** defaults to the value $\chi = 0.01$. The command to specify the convergence tolerance is:

`convergence tolerance` < `number` >

6.5.2.6 Maximum Number of Iterations

Convergence of the iterative procedure generally requires few iterations for common ranges of the tolerance χ. However, in some few cases, the Weibull modulus, m, may oscillate (periodically) around a certain value and convergence of the iterative procedure may not be attained. Users may then define the maximum number of iterations allowed in WSTRESS by using the following command:

`maximum iterations` < `integer` >

6.5.2.7 Effects of Plastic Strain on Cleavage Fracture

WSTRESS provides a simple, but highly effective, model to incorporate the potentially strong effects of plastic strain on cleavage microcracking thereby affecting the cleavage failure probability (see Section 3.5). The approach derives directly from the influence of the effective plastic strain, ϵ_p, on the fraction of eligible Griffith-like microcracks which propagate unstably within the near-tip fracture process zone. A modified form of the Weibull stress, $\tilde{\sigma}_w$, is now introduced by integration of the equivalent (or principal) stress *and* the effective plastic strain over all elements included into the fracture process zone. The input command to include effects of plastic strain effects on the computation of $\tilde{\sigma}_w$ is as follows

$$\texttt{plastic strain (effect)} \begin{cases} \texttt{on} \\ \texttt{off} \end{cases}$$

where the default value is `off`.

Currently, ***WSTRESS*** allows using two models to include effects of plastic strain on the Weibull stress as defined by the fraction of fractured particles, Ψ_c, which trigger unstable (cleavage) fracture (see previous Eqs. (3.11) in Section 3.5): (1) simplified distribution of the particle fracture stress and (2) exponential dependence of eligible Griffith-like microcracks. The command to define the fraction of fractured particles has the form:

$$\texttt{eligible microcrack model} \begin{cases} \texttt{particle fracture stress (distribution)} \\ \texttt{exponential } (\textit{distribution}) \end{cases}$$

Each plastic strain model requires the specification of a set of adequate parameters defining the fraction of fractured particles, Ψ_c. For the simplified distribution of the particle fracture stress, these parameters are the shape parameter of the Weibull distribution for the particle fracture stress, α_p, the elastic modulus of the particle, E_d, the particle shape parameter, β_p and the reference fracture stress of the particle, σ_{prs}. In general, parameters α_p, E_d and β_p are assumed fixed, known quantities at the onset of the analysis with parameter σ_{prs} remaining to be determined from the calibration procedure. For the exponential model to describe the distribution of eligible Griffith-like microcracks, only parameter λ is required and, thus, represents the quantity to be determined from the calibration procedure. The command to specify the parameters defining the fraction of fractured particles has the form:

fractured particle (distribution) parameters ,

  alpha_part < number > beta_part < number > ,

  e_part < number > sigma_part < number >

fractured particle (distribution) parameters lambda < number >

In the above commands, there are no default values assigned to the parameters defining the fraction of fractured particles, Ψ_c. Further, each of the above commands *must follow* the corresponding plastic strain model defining the fraction of eligible microcracks.

6.5.3 Statistical Parameters

The statistical parameters section defines the parameters used directly in the statistical procedures and specifics of the Weibull model. A typical block consists of the following subcommands.

6.5.3.1 Point Estimation Method

The iterative procedure offers two statistical methods for point estimation of the parameters of the Weibull distribution: 1) the maximum likelihood method and 2) least square procedure. The maximum likelihood method yields the best estimates with minimum asymptotic variances (refer to Appendix A) and is the default option in ***WSTRESS***. The default point estimation method is the maximum likelihood procedure. The command to define the point estimation method is:

$$\texttt{estimation method} \begin{cases} \texttt{maximum likelihood} \\ \textit{least square} \end{cases}$$

6.5.3.2 Initial Value of the Weibull Modulus (Shape Parameter)

The iterative procedure outlined in Chapter 4 requires a starting estimate for the Weibull modulus or shape parameter, m. ***WSTRESS*** defaults the initial value of the Weibull modulus to 20. The command syntax is as follows:

initial weibull modulus < number >

6.5.3.3 Reference Volume

WSTRESS assumes a unit volume for the reference volume, V_0, in the computation of the Weibull stress. Users may redefine this quantity using the command:

`reference volume` $<$ `number` $>$

However, as discussed previously, the effect of adopting a different valur for V_0 is simply the scaling of parameter σ_u as the Weibull modulus, m, is independent of V_0 (refer to Section 3.1).

6.5.3.4 Threshold Stress

WSTRESS sets the value of the threshold stress, σ_{th}, appearing in Eq. (3.6) (see Section 3.3) as 0. Different values for σ_{th} can be specified as needed with the following command:

`threshold stress` $<$ `number` $>$

7

Illustrative Example

This section illustrates computation of the Weibull modulus, m, for a low alloy structural steel based upon fracture toughness tests conducted by Barbosa and Ruggieri [78]. Fracture toughness tests were performed on conventional, plane-sided three-point bend fracture specimens with varying crack sizes and specimen thickness in the T-L orientation as illustrated in Fig. 7.1. Testing of these configurations was performed at $T = -20°$C which corresponds to the lower-shelf, ductile-to-brittle transition behavior for the tested steel (refer to Fig. 7.2(b) next). The fracture mechanics tests include conventional, plane-sided 1T SE(B) specimens with $a/W = 0.5$ and $a/W = 0.2$, $B = 25$ mm, $W = 50$ mm and $S = 4W$ loaded under 3-point bending. Here, a is the crack size, W denotes the specimen width, B represents the specimen thickness and S is the load span. ASTM E1820 [79] provides additional details for the geometry and dimensions of the tested fracture specimens. The test matrix also includes testing of plane-sided 0.8T SE(B) specimens with $a/W = 0.5$, $B = 20$ mm, $W = 40$ mm and $6W$ loaded under 3-point and 4-point bending and precracked Charpy specimens (PCVN); however, these specimen geometries are not used for calibration of parameter m in the present example.

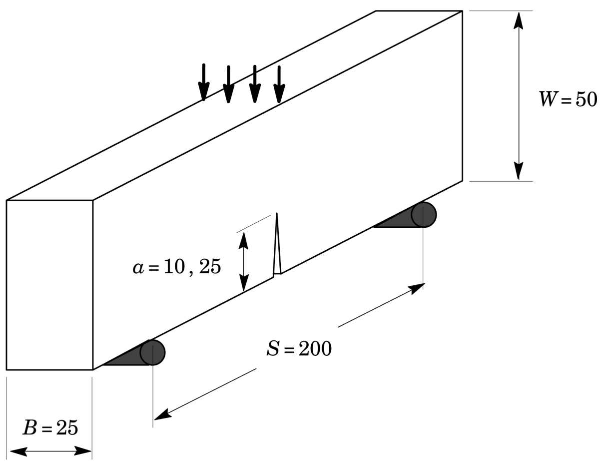

Figure 7.1: *Geometries of the tested SE(B) fracture specimens with* $a/W = 0.5$ *and* $a/W = 0.2$.

The material utilized in this study is a typical ASTM A572 Grade 50 structural steel with 376 MPa yield stress and 555 MPa tensile strength at room temperature (20°) and relatively moderate hardening properties ($\sigma_{uts}/\sigma_{ys} \approx 1.5$, where σ_{ys} is the yield stress and σ_{uts} denotes the ultimate strength). Figure 7.2(a) shows the engineering stress-strain response at room and test (−20°C) temperature. Figure 7.2(b) shows the measured toughness-temperature properties for the material in terms of conventional Charpy-V impact energy (T-L orientation).

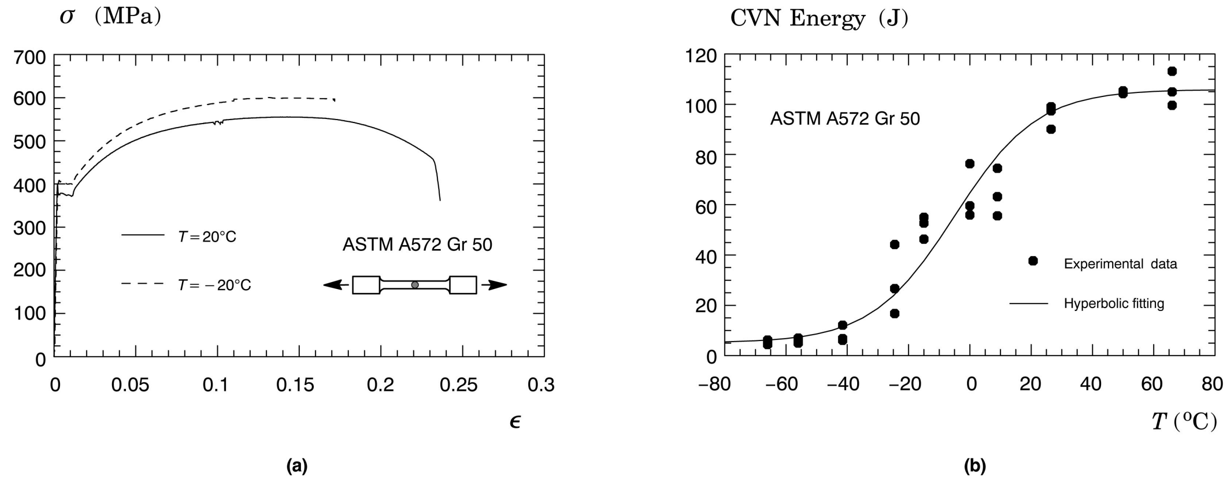

Figure 7.2: *Mechanical properties of tested A572 Gr 50 steel: (a) Engineering stress-strain response at room and test (−20°C) temperature; (b) Charpy-V impact energy (T-L orientation) versus temperature.*

Figure 7.3 shows a Weibull diagram of the measured toughness values for both test temperatures. These J_c-values were determined using revised η-factors provided in Barbosa and Ruggieri[80]. These η-values are based on crack mouth opening displacement (CMOD) using plane-strain finite element analyses of 1T SE(B) specimens with varying crack sizes (as characterized by the a/W-ratio) and different hardening properties. The solid symbols in the plots indicate the experimental fracture toughness data for the specimens. Values of cumulative probability, $F(J_c)$, are obtained by ordering the J_c-values and using $F(J_{c,k}) = (k - 0.3)/(N + 0.4)$, where k denotes the rank number and N defines the total number of experimental toughness values.

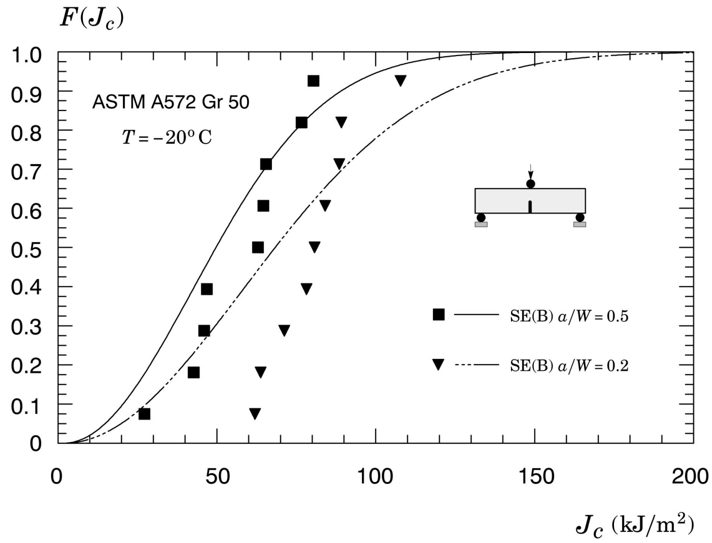

Figure 7.3: *Cumulative probability distribution of measured J_c-values for the tested A572 Gr 50 steel*

The curves displayed in this plot describe the two-parameter Weibull distribution [15] for J_c-values given by

$$F(J_c) = 1 - \exp\left[-\left(\frac{J_c}{J_0}\right)^{\alpha}\right] \tag{7.1}$$

with $\alpha = 2$ (Weibull modulus) and the characteristic toughness, J_0, determined from a maximum likelihood (ML) analysis of the data set [26]. Here, the ML estimates of the Weibull parameters, $(\hat{\alpha},\ \hat{J}_0)$, are $(2.0,\ 59.3\,\mathrm{kJ/m^2})$ for the SE(B) specimen with $a/W = 0.5$ and $(2.0,\ 81.8\,\mathrm{kJ/m^2})$ for the SE(B) specimen with $a/W = 0.2$. In particular, the experimental toughness distribution for the deep crack SE(B) specimen agrees relatively well with the theoretical Weibull distribution described by $\alpha = 2$. Moreover, post-mortem examination of the fracture surfaces for the tested SE(B) specimens revealed essentially no ductile tearing prior to cleavage fracture.

Calibration of the Weibull modulus for the tested structural steel is conducted by performing detailed finite element analyses on 3-D models for the SE(B) specimens. Figure 7.4 shows a typical finite element model constructed for the 3-D analyses of the SE(B) specimen with $a/W = 0.5$. A conventional mesh configuration having a focused ring of elements surrounding the crack front is used with a small key-hole at the crack tip where the radius of the key-hole, ρ_0, is 0.0025 mm. Symmetry conditions permit modeling of only one-quarter of the specimen with appropriate constraints imposed on the remaining ligament and symmetry planes. A typical quarter-symmetric, 3-D model has 34 variable thickness layers with $\sim 41,000$ 8-node, 3-D elements ($\sim 46,000$ nodes) defined over the half-thickness $B/2$; the thickest layer is defined at $Z = 0$ with thinner layers defined near the free surface ($Z = B/2$) to accommodate the strong Z variations in the stress distribution. The finite element models are loaded by displacement increments imposed on the loading points to enhance numerical convergence with increased levels of deformation. The numerical computations for the cracked configurations at the test temperature reported here are generated using the research code WARP3D [27]. The analyses utilize an elastic-plastic constitutive model with flow theory and conventional Mises plasticity in large geometry change (LGC) setting. The true stress-logarithmic strain behavior for the tested material follows a piecewise linear approximation to the measured response shown in Fig. 7.2(a).

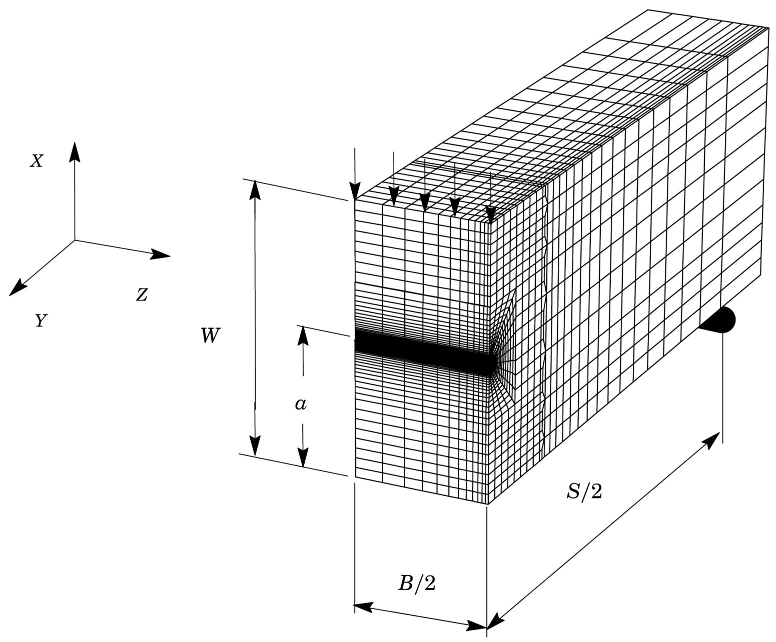

Figure 7.4: *3-D finite element model for the deeply-cracked bend specimen.*

The input parameters, specification of blocks of commands for ***WSTRESS*** are shown next in Fig. 7.5. The procedure to find the material dependent value for the shape parameter, m, is fully described in Chapter 4. For the tested A572 Gr 50 steel, m has the calibrated value of 14.7 using the standard (Beremin) Weibull stress formulation (*i.e.,* with no plastic strain effects included in the calibration procedure).

```
c
c       WSTRESS INPUT FILE
c
c   Calibration of the Weibull Modulus for an A572 structural steel
c   using cleavage fracture toughness data from deep notch and
c   shallow notch SE(B) specimens at -20C tested by Barbosa and Ruggieri
c   (Engineering Fracture Mechanics, Vol. 195, 2018)
c
c   Large Strain Analysis with Key-Hole Crack Tip (0.0025 mm)
c
c
 wstress analysis type parameter calibration
c
  material properties
c
     material a572 {
        yield stress   409 ! yield point at test temperature
        young modulus  201000
        poisson ratio  0.3 }
c
c
  crack configuration sebaw5_B25mm
c
     model definition {
        symmetry factor 4 ! quarter-symmetric model
        get files from directory sebaw5_B25mm
        input mesh from file sebaw5_B25mm_coor
        assign elements 1-41106  material a572
        input loading parameter from file sebaw5_B25mm_a572_jvalues
        format fe-results warp3d patran type ascii
        element type l3disop order 2x2x2 }
c
     experimental data {
         27 65 80 77 43 63 46 65 47 }
c
c
  crack configuration sebaw2_B25mm
c
     model definition {
        symmetry factor 4 ! quarter-symmetric model
        get files from directory sebaw2_B25mm
        input mesh from file sebaw2_B25mm_coor
        assign elements 1-40834  material a572
        input loading parameter from file sebaw2_B25mm_a572_jvalues
        format fe-results warp3d patran type ascii
        element type l3disop order 2x2x2 }
c
     experimental data {
         81 78 71 84 64 89 89 108 62  }
c
c
  analysis parameters
c
     fracture process zone {
      active process zone principal stress
      fracture criterion principal stress
      process zone size parameter 2.0 }
c
     solution parameters {
       warp3d release v18
       parameter calibration on
       loading parameter j-integral
       compute steps for structure sebaw5_B25mm  20-1000 by 20
       compute steps for structure sebaw2_B25mm  20-600 by 20
       convergence tolerance 0.01
       maximum iterations 100
       plastic strain effect off }
c
     statistical parameters {
       initial shape parameter 10
       reference volume 1.0
       threshold stress 0
       estimation method mlh }
c
c
 end
c
```

Figure 7.5: ***WSTRESS*** *input file for the computation of the Weibull modulus, m, for an ASTM A572 Gr 50 steel based upon fracture toughness tests conducted by Barbosa and Ruggieri [78]*

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Appendix A

Point Estimation Using the Maximum Likelihood Method

This section provides details of the maximum likelihood (ML) method implemented in ***WSTRESS*** for statistical inference of the parameters that describe the Weibull distribution for the toughness values (K_{Jc}, J_c or CTOD (δ_c)). Within the framework of parametric models, such as the Weibull model, a number of other estimation procedures are also suitable for determining the estimates of the (unknown) parameters. Classical inference procedures include the method of moments, the least square method and the best linear invariant method - see more specific literature, such as Mann et al. [26], Kendall and Stuart [70] or Bain [81], on the statistical and convergence properties of such methods. Likelihood-based methods are generally simple to implement and provide (theoretically) efficient parameter estimates. The maximum likelihood estimates (MLEs) often satisfy some of the optimality criteria for statistical inferences and are asymptotically unbiased and asymptotically efficient as the number of observations (sample size) increases.

A.1 The Maximum Likelihood Method

Without making recourse to more formal statistical concepts, let $(x_1,\ x_2,\ \ldots,\ x_n)$ with $x_i \leq x_{i+1}$ denote an independent and identically distributed ordered sample of size n from the population of interest; without loss of generality, the random variable X_i is associated with the toughness values, $J_{c,i}$ and the corresponding $\sigma_{w,c,i}$-values in the present work. Now define the probability density function, referred to as *pdf*, in the form $f(x,\ \xi)$ where the parameter vector $\xi = (\xi_1, \ldots, \xi_m)$ is unknown. For the set of observations x_i, the likelihood function $L(\xi)$ is defined as the joint density of the n random variables in the form

$$L(\xi) = \prod_{i=1}^{n} f(x_i,\ \xi) \quad . \tag{A.1.1}$$

The maximum likelihood estimates (MLEs) $(\hat{\xi}_1, \ldots, \hat{\xi}_m)$ of $(\xi_1, \ldots, \xi_m)$ are those values that maximize the likelihood function, or equivalently, the log-likelihood form of Eq. (A.1.1) defined by

$\ln L(\xi)$. Hence, the MLEs are simply determined by solving the following set of likelihood equations

$$\frac{\partial \ln L(\xi)}{\partial \xi_j} = 0 \quad , \quad j = 1,\, 2, \ldots,\, m \quad . \tag{A.1.2}$$

Fracture mechanics data upon which the method of estimation is based may sometimes contain *incomplete* observations, which are referred to as *censored* observations [26, 81, 82]. In the present context, a common form of incomplete observations is related to cleavage fracture toughness data exhibiting two types of fracture modes: perfect cleavage (stable crack growth prior to failure is negligible, *e. g.*, $\Delta a \leq 0.1 \sim 0.2$mm) and cleavage after some amount of ductile tearing (which may exceed several times the CTOD value at onset of crack growth, δ_{Ic}). Another case of considerable interest refers to cleavage fracture toughness data sets in which some of the toughness values exceed the measuring capacity of the tested specimens for fracture toughness prior to constraint loss as characterized by the deformation limit expressed by $M = b\sigma_{ys}/J$, with M typically assigned values of $30 \sim 60$. For example, the procedure to characterize fracture toughness data over the DBT region, known generally as the "Master Curve" methodology and standardized as ASTM E1921 [83], adopts a deformation limit of $M = 30$ to characterize fracture toughness values under high constraint (triaxiality) condition of plane-strain, small-scale yielding (SSY) with a T-stress ≥ 0 [76]. Consequently, cleavage fracture toughness data for typical ferritic steels tested in the DBT region may also exhibit incomplete observations in which a number of fracture toughness values satisfy the condition $M > 30$ whereas the remaining of the fracture toughness values exceeds the deformation limit, given by $M \leq 30$.

WSTRESS analyses incomplete fracture toughness data sets by using a censoring procedure known as a Type I censoring model. Let again $(x_1,\, x_2,\, \ldots,\, x_n)$ with $x_i \leq x_{i+1}$ denote an independent and identically distributed ordered sample of size n from the population of interest. Also, let x_s be some (preassigned) fixed value termed the *fixed censoring parameter*. Instead of observing $(x_1,\, x_2,\, \ldots,\, x_n)$ (the random variable of interest), we can only observe $(y_1,\, y_2,\, \ldots,\, y_n)$ where

$$y_i = \begin{cases} x_i & ; \quad x_i \leq x_s \quad , \quad i = 1, \ldots,\, r \\ x_r & ; \quad x_i > x_r \quad , \quad i = r+1, \ldots,\, n \end{cases} \tag{A.1.3}$$

so that there are r uncensored observations $(x_i \leq x_r)$ and $n - r$ censored observations $(x_i > x_r)$. Note that for the censoring mechanism adopted, r also becomes a random variable. Then the likelihood function, $L(\xi)$, is now given by

$$L(\xi) = \prod_{i=1}^{r} f(x_i,\, \xi) \prod_{j=r+1}^{n} S(x_j,\, \xi) \tag{A.1.4}$$

where $S(x,\, \xi)$ is the survivor (or reliability) function with respect to the random variable X. Since it is understood that when $n = r$ the last product in the above Eq. (A.1.4) is not involved, this expression may be viewed as a more *general* likelihood equation and it is the one implemented in ***WSTRESS***.

A.2 Maximum Likelihood Estimates for the Weibull Distribution

For the two-parameter Weibull distribution of J_c given by previous Eq. (2.2), the probability density function is written as

$$f(J_c) = \alpha J_0^{-\alpha} J_c^{\alpha-1} \exp\left[-\left(\frac{J_c}{J_0}\right)^{\alpha}\right] \quad , \quad J_c > 0 \tag{A.2.1}$$

and the survivor function is

$$S(J_c) = \exp\left[-\left(\frac{J_c}{J_0}\right)^{\alpha}\right] \quad , \quad J_c > 0 \tag{A.2.2}$$

where $\alpha > 0$ and $J_0 > 0$ are the Weibull modulus and scale parameter, respectively.

The Weibull distribution represents one of the most widely distributions used in reliability analysis and probabilistic fracture mechanics. The strength of this models lies in its flexible shape for describing many failure mechanisms with a wide variety of possible failure rates. In addition, the Weibull model is directly connected to a type III extreme value distribution [25, 26], which also suggests its theoretical applicability when failure is due to weakest link mechanisms. The Weibull modulus, α, plays the major role in determining the shape of the distribution. In the present context, α describes the scatter of the data set (the set of observations $J_{c,i}$). The scale parameter, J_0, represents the characteristic value of the fracture toughness data set, $J_{c,i}$ (which can be associated with a *characteristic toughness* in the present framework) and corresponds to the 63.2 percentile on the cumulative distribution function. The scale parameter also gives an approximate measure for the media value of the observations, J_{c-med}, since $J_{c-med} \approx 0.9124 J_0$ [26].

Another interpretation on the significance of the Weibull parameters, particularly the Weibull modulus, follows from the concept of *hazard* or *failure rate* function of the time-to-failure random variable T (see Mann, et al. [26] or Kapur and Lamberson [84]), denoted as $h(t)$. Let $F(t)$ be the distribution function of T and $f(t)$ its probability density function. Then, the hazard rate is defined as

$$h(t) = \frac{f(t)}{1 - F(t)} \tag{A.2.3}$$

where $1 - F(t)$ is the reliability or survival function, also denoted as $S(t)$. The probabilistic interpretation of $h(t)$ is as follows. The hazard function represents the conditional probability that a unit fails at time $t + \Delta t$ given that it has not failed at time t. Within the present methodology, increasing "time" can be replaced by increasing crack-tip "damage". The hazard function is an indicator of the "proneness to failure" of a unit after surviving until time t. In the Weibull model, the modulus α has a close correlation with the failure rate of the physical process. When $\alpha = 1$, the Weibull distribution reduces to the exponential distribution and the failure rate, $h(t)$, is constant. When $\alpha < 1$, the failure rate decreases with increasing material damage. When $\alpha > 1$, the failure rate increases with increased material damage. In the light of these observations, it is argued that the Weibull modulus, α, can never be ≤ 1 to describe the toughness distribution for cleavage fracture data. Otherwise, near-tip damage would increase with increased remote lading (as measured by J) but the failure rate would decrease. One could also argue that values of α less than about 2 for fracture toughness data (J_c or δ_c) are also not very representative of cleavage fracture as the failure rate, though an increasing function of damage, would increase very slowly.

Now, for computational convenience, it is useful to adopt the parametrization $\gamma = J_0^{-\alpha}$ so that Eq. (A.2.1) and (A.2.2) are rewritten in the form

$$f(J_c) = \alpha\gamma J_c^{\alpha-1} \exp\left(-\gamma J_c^{\alpha}\right) \tag{A.2.4}$$

and

$$S(J_c) = \exp\left(-\gamma J_c^{\alpha}\right) \tag{A.2.5}$$

from which the likelihood equation described by Eq. (A.1.4) for the Weibull distribution is given by

$$L(\alpha, \gamma) = (\alpha\gamma)^r \prod_{i=1}^{r} J_{c,i}^{\alpha-1} \exp\left[-\gamma \sum_{i=1}^{r} J_{c,i}^{\alpha}\right] \exp\left[-\gamma(n-r)J_r^{\alpha}\right] \tag{A.2.6}$$

where J_r is now the censoring parameter associated with the toughness data set, $J_{c,i}$. As described previously, the maximum likelihood estimates (MLEs) defined by $(\hat{\alpha},\, \hat{\gamma})$ (or, equivalently, $(\hat{\alpha},\, \hat{J}_0)$) are found by maximizing the log-likelihood form of this expression - see Eq. (A.1.2). This operation defines a set of two equations in terms of the variables $(\alpha,\, \gamma)$ which must be solved iteratively as described next. The likelihood function previously described remains equally valid for any threshold value, $J_{min} > 0$ by an appropriate transformation of data in the form $\tilde{J}_{c,i} = J_{c,i} - J_{min}$.

Evaluation of the fixed censoring parameter, J_r, represents an important step in estimating the parameters $(\hat{\alpha},\, \hat{\gamma})$ or, equivalently, $(\hat{\alpha},\, \hat{J}_0)$ for the Type I censoring model. For the previous example, *i.e.*, fracture displaying two failure modes (perfect cleavage and cleavage after stable ductile extension), Minami, et al. [18] adopted the value of J (or, equivalently, the CTOD) at ductile crack initiation, J_{Ic}. A reasonable estimate for the fixed censoring parameter would also be the average value between the *largest* J_c-value for the data set exhibiting only cleavage and the *smallest* J_c-value for the data set exhibiting cleavage after ductile tearing. For small sample sizes, however, the MLEs may show strong sensitivity to the choice of the fixed censoring parameter, J_r.

A.3 Solution of the Likelihood Equations

This section provides further details of the procedure to determine the MLEs for the parameters of the Weibull distribution given by Eq. (2.2) described by the Weibull modulus, α, and the scale parameter, J_0. Recalling the parametrization $\gamma = J_0^{-\alpha}$ introduce above, the log-likelihood function, Eq. (A.2.6), is given by

$$\Upsilon = \ln L(\alpha,\, \gamma) = r \ln \gamma + r \ln \alpha + (\alpha - 1) \sum_{i=1}^{r} \ln y_i - \gamma \sum_{i=1}^{n} y_i^{\alpha} \tag{A.3.1}$$

where the random variable of interest, $(y_1, \ldots,\, y_n)$ is defined previously by Eq. (A.1.3) so that there are r uncensored observations $(x_i \leq x_r)$ and $n - r$ censored observations $(x_i > x_r)$ with x_r denoting the censoring parameter. Here, it is understood that $y_1 \equiv J_{c,1},\, y_2 \equiv J_{c,2},\, \ldots,\, y_n \equiv J_{c,n}$ (or, equivalently, $\delta_{c,n}$ or $K_{Jc,n}$).

Taking the first derivatives of the above Eq. (A.3.1) with respect to α and γ yields

$$\frac{\partial \Upsilon}{\partial \alpha} = \frac{r}{\alpha} - \sum_{i=1}^{r} y_i - \gamma \sum_{i=1}^{n} y_i^{m} \ln y_i \quad , \tag{A.3.2}$$

$$\frac{\partial \Upsilon}{\partial \gamma} = \frac{r}{\gamma} - \sum_{i=1}^{n} y_i^{m} \quad . \tag{A.3.3}$$

Setting these equations to zero, the MLEs $(\hat{\alpha},\, \hat{\gamma})$ satisfy

$$\frac{r}{\alpha} - \sum_{i=1}^{r} y_i - \gamma \sum_{i=1}^{n} y_i^{m} \ln y_i = 0 \quad , \tag{A.3.4}$$

$$\frac{r}{\gamma} - \sum_{i=1}^{n} y_i^{m} = 0 \quad . \tag{A.3.5}$$

so that the likelihood estimate for the Weibull modulus, $\hat{\alpha}$, is found by solving

$$\frac{r}{\alpha} - \sum_{i=1}^{n} y_i - r \left[\left(\sum_{i=1}^{n} y_i^{\alpha} \ln y_i \right) / \sum_{i=1}^{n} y_i^{\alpha} \right] = 0 \tag{A.3.6}$$

which can be solved iteratively by a convenient numerical procedure such as the Newton method [77].

A.4 Random Generation of Fracture Data

The numerical strategy to calibrate the Weibull stress parameter, $(m,\, \sigma_u)$ described in previous Section 4.3) utilizes measured toughness data for cleavage fracture, J_c or δ_c. Alternatively, the statistical sample of fracture toughness data can be generated from a specified Weibull distribution in which parameters $(\alpha,\, J_0)$ are known at the onset of the analysis. Generation of fracture data offers significant advantages when users want to incorporate a fixed set of Weibull parameters representing the cleavage fracture process of a particular material into the procedure to estimate the Weibull stress parameter, $(m,\ \sigma_u)$.

To generate a statistical sample for J_c, denoted by $J_{c,gen}$, corresponding to the three-parameter Weibull distribution defined by previous Eq. (2.1), a Monte Carlo simulation with inverse transformation method [26] is employed in the form

$$J_{c,gen} = J_0 \left[-\ln(1-U)\right]^{1/\alpha} + J_{min} \tag{A.4.1}$$

where U is uniformly distributed between [0, 1]. ***WSTRESS*** utilizes a random number generator which reflects a linear congruential procedure [77] to produce the uniformly distributed random variate, U, in the unit interval. A large data set for $J_{c,gen}$ (usually with more than 10000 points) is then generated using Eq. (A.4.1) to guarantee sufficient accuracy in the simulation process of the probability distribution.