Fracture Toughness Predictions Using the Weibull Stress Model with Implications for Estimations of the T_0 Reference Temperature

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Abstract This work presents a numerical and experimental investigation into the applicability of precracked Charpy specimens to determine the T_0 reference temperature for pressure vessel steels. A central objective is evaluate the effectiveness of the Weibull stress model to correct effects of constraint loss in PCVN specimens which serves to determine the indexing temperature T_0 based on the Master Curve methodology. Fracture toughness testing conducted on an A285 Grade C pressure vessel steel provides the cleavage fracture toughness data needed to estimate T_0. For the tested material, the Weibull stress methodology yields estimates for the reference temperature from small fracture specimens which are in good agreement with the corresponding estimates derived from testing of much larger crack configurations.

Keywords Cleavage Fracture, Constraint Effects, Weibull Stress, Master Curve, PCVN Specimen

1. Introduction

Standard compact tension and three-point bend specimens containing deep, through cracks ($a/W \geq 0.5$) are commonly employed in fracture toughness testing of ferritic steels in the ductile-to-brittle transition (DBT) region. The primary motivation to use deeply cracked specimens is to guarantee SSY conditions leading to high crack-tip constraint with limited-scale plasticity. Under these conditions, fracture toughness values (such as the J-integral at cleavage instability, J_c, or the elastic-plastic stress intensity factor, K_{Jc}) prove effective to characterize the essentially stress-controlled failure by a transgranular cleavage mechanism.

Current structural integrity assessment procedures for reactor pressure vessels (RPVs) focus on the utilization of small fracture specimens to facilitate experimental measurements of fracture toughness data. In particular, three-point bend testing of precracked Charpy (PCVN) specimens become necessary when severe limitations exist on material availability, for example, in nuclear irradiation embrittlement studies, as this specimen configuration is predominant within surveillance capsule programs. However, the measuring capacity of these specimens for fracture toughness prior to constraint loss may be insufficient for moderate strength pressure vessel and structural steels. Once constraint loss occurs, measured values of cleavage fracture toughness (J_c, K_{Jc}) increase markedly as the global plastic deformation interacts with the local crack front fields (governed by J) thereby relaxing the level of stress triaxiality. Moreover, cleavage fracture is a highly localized phenomenon which exhibits strong sensitivity to material characteristics at the microlevel. In particular, the random inhomogeneity in local features of the material causes large scatter in measured values of cleavage fracture toughness. The coupled effects of constraint loss and inherent scatter of toughness values in the DBT region greatly complicate the development of fracture mechanics assessments based on small specimen data.

Motivated by these observations, this work explores application of a micromechanics model to determine the T_0 reference temperature for pressure vessel steels from precracked Charpy (PCVN) specimens. A central objective is evaluate the effectiveness of the Weibull stress model to correct effects of constraint loss in PCVN specimens which serves to determine the indexing temperature T_0 based on the Master Curve methodology. Fracture toughness testing conducted on an A285

Grade C pressure vessel steel provides the cleavage fracture toughness data needed to estimate T_0. For the tested material, the Weibull stress methodology yields estimates for the reference temperature, T_0, from small fracture specimens which are in good agreement with the corresponding estimates derived from testing of much larger crack configurations.

2. Overview of the Weibull Stress Model for Cleavage Fracture

2.1. Weakest Link Modeling of Cleavage Fracture

Extensive work on cleavage fracture in ferritic steels demonstrates that cracking of grain boundary carbides in the course of plastic deformation and subsequent extension of these cracks into the surrounding matrix governs failure. The inherent random nature of failure micromechanism causes large scatter in the measured values of cleavage fracture toughness for ferritic steels tested in the DBT region thereby complicating quantitative assessments of fracture behavior in terms of meaningful toughness values. A continuous probability function derived from weakest link statistics conveniently characterizes the distribution of toughness values, described by J_c-values, as [1]

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

which is a three-parameter Weibull distribution with parameters (α, J_0, J_{th}). Here, α denotes the Weibull modulus (shape parameter), J_0 defines the characteristic toughness (scale parameter) and J_{th} is the threshold fracture toughness. Often, the threshold fracture toughness is set equal to zero so that the Weibull function given by Eq. (1) assumes its more familiar two-parameter form. The above limiting distribution remains applicable for other measures of fracture toughness, such as K_{Jc} or δ (CTOD). Under SSY conditions, the scatter in cleavage fracture toughness data is characterized by $\alpha = 2$ for J_c-distributions or $\alpha = 4$ for K_{Jc}-distributions [2].

A number of micromechanics models to describe transgranular cleavage, most derived from the *local approach* philosophy, have focused on probabilistic methodologies which couple the micromechanical features of the fracture process with the inhomogeneous character of the near-tip stress fields. By adopting weakest link arguments to describe the failure event, the overall fracture resistance is assumed to be driven by the largest fracture-triggering particle that is sampled in the fracture process zone ahead of crack front. This approach enables defining a probability distribution for the fracture stress of a cracked solid with increased loading (represented by the *J*-integral) in terms of a two-parameter Weibull distribution [3-5] in the form

$$P(\sigma_w) = 1 - \exp\left[-\frac{1}{\Omega_0} \int_{\Omega} \left(\frac{\sigma_1}{\sigma_u} \right)^{m} d\Omega \right] = 1 - \exp\left[-\left(\frac{\sigma_w}{\sigma_u} \right)^{m} \right] \quad , \quad \sigma_1 \geq 0 \tag{2}$$

where Ω denotes the volume of the (near-tip) fracture process zone, Ω_0 represents a (unit) reference volume and σ_1 is the maximum principal stress acting on material points inside the fracture process zone. In the present work, the active fracture process zone is defined as the loci where $\sigma_1 \geq \lambda \sigma_{ys}$, with $\lambda \approx 2 \sim 2.5$ and σ_{ys} represents the material's yield stress. Parameters *m* and σ_u appearing in Eq. (2) denote the Weibull modulus and the scale parameter of the Weibull distribution. The stress integral appearing in Eq. (2) defines the Weibull stress, σ_w, a term coined by the Beremin group [3], in the form

$$\sigma_w = \left[\frac{1}{\Omega_0} \int_\Omega \sigma_1^m d\Omega \right]^{1/m} \quad , \quad \sigma_1 \geq 0 \tag{3}$$

A central feature of this methodology involves the interpretation of σ_w as a macroscopic crack driving force [4-5]. Consequently, it follows that unstable crack propagation (cleavage) occurs at a critical value of the Weibull stress; under increased remote loading (as measured by *J*), differences in evolution of the Weibull stress reflect the potentially strong variations of near-tip stress fields

2.2. Effects of Plastic Strain on the Probabilistic Crack Driving Force

The previous approach can be further extended to include the strong effects of near-tip plastic strain on cleavage microcracking thereby altering the microcrack distribution entering into the local criterion for fracture. Based upon direct observations of cleavage microcracking by plastic strain made in ferritic steels at varying temperatures [6-8], a *generalized* form of the Weibull stress can be defined as

$$\sigma_w = \left[\frac{1}{\Omega_0} \int_\Omega \varepsilon_p^{\gamma(1+\beta)} \sigma_1^m d\Omega \right]^{1/m} \quad , \quad \sigma_1 \geq 0 \tag{4}$$

Here, $\varepsilon_p = f(J)$ is the near-tip effective plastic strain, and γ and β are parameters defining the contribution of the plastic strain on cleavage fracture probability; for example, setting $\gamma = 0$ recovers the conventional description for the probability distribution of fracture stress. The above plastic term correction simply reflects the increase in cleavage fracture probability that results from the growth in microcrack density with increased levels of near-tip plastic strain. Ruggieri [5] provides further details on the character of the previous definition for the generalized Weibull stress.

Early work of the Beremin group [3] also recognized the potential strong effects of plastic deformation on cleavage fracture. Based on experimental analyses of the failure strain for notched specimens made of an ASTM A508 steel, they proposed a modified form of previous Eq. (3) as

$$\sigma_w = \left[\frac{1}{\Omega_0} \int_\Omega \exp\left(-\frac{m\varepsilon_p}{2} \right) \sigma_1^m d\Omega \right]^{1/m} \quad , \quad \sigma_1 \geq 0 \tag{5}$$

which indicates that σ_w increases approximately with $\exp(\varepsilon_p/2)$.

3. Summary of the Master Curve Approach

Wallin [9] has developed a relatively straightforward procedure to characterize fracture toughness data over the DBT region, widely known as the *master curve approach*, which relies on the concept of a normalized curve of median fracture toughness *vs.* temperature applicable to hold experimentally for a wide range of ferritic pressure vessel and structural steels. The approach begins by adopting a three-parameter Weibull distribution to describe the distribution of toughness values in the form

$$F\left(K_{Jc}\right)=1-\exp\left[-\left(\frac{K_{Jc}-K_{\min}}{K_0-K_{\min}}\right)^{\alpha}\right] \tag{6}$$

where the Weibull modulus, α, takes the value of 4.

Now, following a standard maximum likelihood estimate, the scale parameter, K_0, corresponding to the 63.2% cumulative failure probability, is given by

$$K_0=\left[\sum_{i=1}^{N}\frac{\left(K_{Jc(i)}-20\right)^4}{\left(r-0.3068\right)}\right]^{1/4}+20 \qquad \text{MPa}\sqrt{\text{m}} \tag{7}$$

where N denotes the total number of specimens tested and r represents the number of valid tests (uncensored data). The median toughness at the tested temperature follows simply as

$$K_{Jc(med)}=0.9124\left(K_0-20\right)+20 \qquad \text{MPa}\sqrt{\text{m}} \tag{8}$$

The *master curve* of median toughness, $K_{Jc(med)}$, for 1-T specimens over the transition range for the material has the final form

$$K_{Jc(med)}=20+70\exp\left[0.019\left(T-T_0\right)\right] \qquad {}^{\circ}\text{C},\ \text{MPa}\sqrt{\text{m}} \tag{9}$$

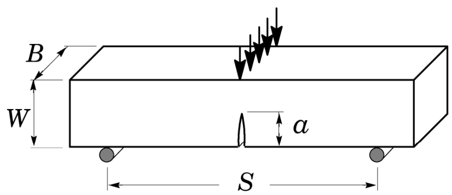
where T is the test temperature and T_0 is the reference (indexing) temperature The above expression for the median toughness applies throughout the lower part of the DBT range prior to the occurrence of significant ductile tearing. ASTM E1921 [10] test standard outlines procedures to construct various tolerance bounds based on the above representation for the toughness distribution.

4. Computational Procedures and Finite Element Models

Calibration of the Weibull modulus for the tested pressure vessel steel is conducted by performing detailed finite element analyses on 3-D models for the SE(B) and precracked Charpy specimens. described in Section 5.1. The analysis matrix includes conventional, plane-sided SE(B) specimens with $a/W=0.2$ and 0.5, and precracked Charpy (PCVN) specimens with $a/W=0.5$.

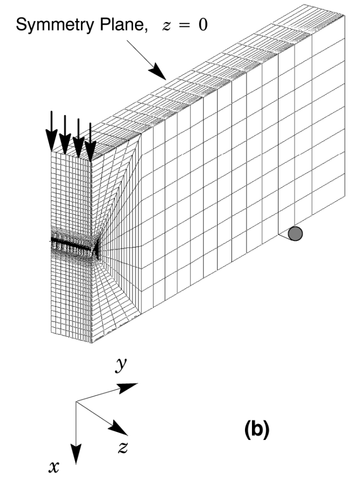
Figure 1 shows a typical finite element model constructed for the 3-D analyses of the SE(B) specimen with $a/W=$ 0.5. A conventional mesh configuration having a focused ring of elements surrounding the crack front is used with a small key-hole at the crack tip where the radius of the key-hole, ρ_0, is 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 22 variable thickness layers with ~27000 8-node, 3-D elements (~31000 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 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 next section addresses cleavage fracture predictions using the Weibull stress model based on toughness data measured at different lower-shelf temperatures. The numerical computations for the cracked configurations at the test temperature reported here are generated using the research code WARP3D [11]. The analyses utilize an elastic-plastic constitutive model with J_2 flow theory and conventional Mises plasticity in large geometry change (LGC) setting. The plastic stress-strain response for the tested material follows a power hardening law given by $\varepsilon/\varepsilon_{ys} \propto (\sigma/\sigma_{ys})^n$ where n denotes the strain hardening exponent, σ_{ys} and ε_{ys} are the (reference) yield stress and strain. Using the tensile properties provided in Savioli and Ruggieri [12] and an improved estimate for the hardening exponent given by API 579 [13], the strain hardening exponents yield $n = 6.3$ at $T = -80°C$ and $n = 5.2$ at $T = -60°C$.



(a)

Specimen	B	W	a	a/W	S
SE(B) 1-T $a/W = 0.2$	25	50	10	0.2	200
SE(B) 1-T $a/W = 0.5$	25	50	25	0.5	200
PCVN	10	10	5	0.5	40



(b)

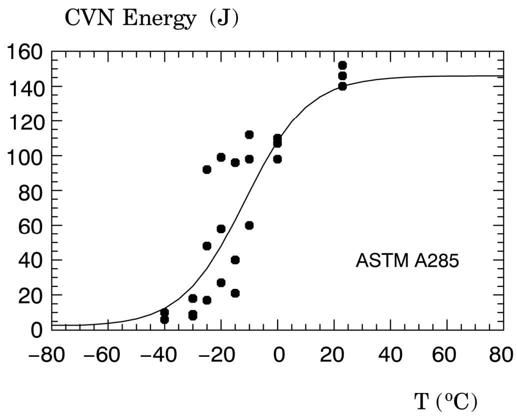
Figure 1. Fracture specimens utilized in the analyses (all dimensions in mm).

5. Cleavage Fracture Predictions

5.1. Mechanical Properties and Experimental Toughness Data for Tested Material

A series of toughness tests was conducted on bend fracture specimens made of a C-Mn low alloy pressure vessel steel in the T-L orientation. The fracture mechanics tests include: (1) conventional, plane sided SE(B) specimens with $a/W = 0.2$ and 0.5, $B = 25$ mm, $W = 50$ mm and $S = 4W$ and (2) a precracked Charpy specimen with $a/W = 0.5$, $B = 10$ mm, $W = 10$ mm and $S = 4W$. Testing of these configurations was performed at $T = -80°C$ for the deeply-cracked SE(B) specimen and PCVN specimens and $T = -60°C$ for the shallow-cracked SE(B) specimen; these temperatures correspond to the lower-shelf, ductile-to-brittle transition behavior for the tested steel. Figure 2(a) shows the measured toughness-temperature properties for the material in terms of conventional Charpy-V impact energy (T-L orientation).

The material is an ASTM A285 Grade C pressure vessel steel with 230 MPa yield stress at room temperature (20°C) and high hardening properties ($\sigma_{uts}/\sigma_{ys} \approx 2.36$). Figure 2(b) shows the engineering stress-strain response at room temperature. Additional tensile tests were conducted at $T = -60°C$ and $-80°C$ to measure the flow properties utilized in the finite element analyses of the fracture specimens described previously. Savioli and Ruggieri [12] provide the measured mechanical properties at different temperatures.



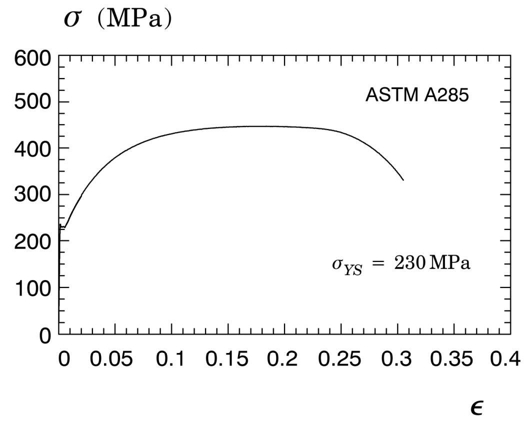


Figure 2. Mechanical properties of the tested A285 Gr C steel: (a) Charpy-V impact energy (T-L orientation) versus temperature; (b) Engineering stress-strain response at room temperature.

Figure 3 provides a Weibull diagram of the measured toughness values for both test temperatures. These J_c-values were determined using revised η-factors based on crack mouth opening displacement (CMOD) recently developed by Ruggieri [14] using full 3-D finite element analyses of 1-T SE(B) specimens and PCVN configurations with varying crack sizes (as characterized by a/W) 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. The curves displayed in this plot indicate the two-parameter Weibull distribution, Eq. (1), obtained by a maximum likelihood analysis of the data set with $\alpha = 2$. Here, the maximum likelihood estimates of the Weibull parameters, $(\hat{\alpha}, \hat{J}_0)$, are $(2.0, 72.6\,\mathrm{kJ/m^2})$ for the SE(B) specimen with $a/W = 0.5$, $(2.0, 215.2\,\mathrm{kJ/m^2})$ for the SE(B) specimen with $a/W = 0.2$ and $(2.0, 217.8\,\mathrm{kJ/m^2})$ for the PCVN configuration. In particular, the experimental toughness distribution for the deep crack SE(B) specimen agrees very well with the theoretical Weibull distribution.

5.2. Determination of T_0 and Master Curve Analysis

The master curve analysis described here followed the procedures of ASTM 1921 [10] summarized previously. The reference temperature was estimated from the toughness distribution of J_c-values at $T = -80°\mathrm{C}$ converted to K_{Jc}-values using $K_{Jc} = \sqrt{EJ_c/(1-\nu^2)}$, where plane-strain conditions are assumed. For the tested pressure vessel steel, the indexing (reference) temperature has the value of $T_0 = -93.5\,^{\circ}\mathrm{C}$.

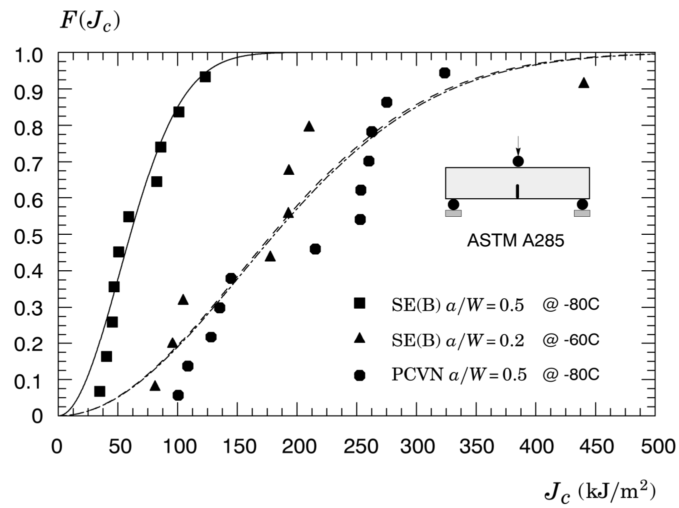


Figure 3. Two-parameter Weibull distribution of experimentally measured J_c-values.

5.3. Calibration of Weibull Stress Modulus

The parameter calibration scheme described in Gao et al. [15] and Ruggieri [5] is applied to determine the Weibull stress parameters for the tested pressure vessel steel. The Weibull modulus, *m*, is calibrated using the SE(B) specimens. Because these specimens were not tested at the same temperature, the present methodology adopts a simple procedure to correct the measured toughness values for temperature in which the J_c-values for the deep crack SE(B) specimens ($a/W = 0.5$) at $T = -80$°C are scaled to corresponding J_c-values at $T = -60$°C using the Master Curve fitting obtained previously. The characteristic toughness values for the deep notch and shallow notch SE(B) specimens are then given as: $J_0 =$ 116.5 KJ/m^2 and 215.2 KJ/m^2.

With the toughness values for the deep and shallow crack SE(B) specimens set at the same temperature ($T = -60$°C) and using σ_w *vs.* J curves constructed from the 3-D finite element analyses for both crack configurations, the calibration procedure is then applied to determine the *m*-value that yields the best correction $J_0^{SE(B)_{a/W=0.5}} \rightarrow J_0^{SE(B)_{a/W=0.2}}$. Table 1 provides the calibrated Weibull stress modulus, *m*, for the tested material based on different definitions for σ_w: 1) $\gamma = 0$ (no plastic strain correction); 2) $\gamma = 1$ and $\beta = 0$ (linear plastic strain correction); 3) $\gamma = 1/2$ and $\beta = 0$ (square root plastic strain correction) and 4) Beremin plastic strain correction.

Table 1. Calibrated Weibull parameter, *m*, for different forms of σ_w

Weibull Stress Model	***m***
Standard Beremin ($\gamma = 0$ with no plastic strain correction)	10.4
Generalized Weibull Stress with $\gamma = 1$ and $\beta = 0$ (linear correction)	28.5
Generalized Weibull Stress with $\gamma = 1/2$ and $\beta = 0$ (square root correction)	28.0
Plastic Strain Modified Beremin Model	29.0

5.4. Cleavage Fracture Predictions Using the Weibull Stress Model

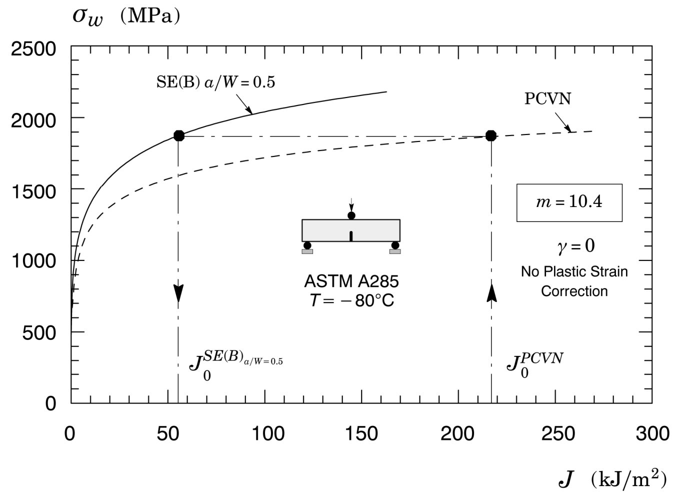
The procedure used here to predict the effects of constraint loss for the experimental cleavage fracture toughness data follows the toughness scaling model introduced by Ruggieri and Dodds [4]. Based upon micromechanics considerations, the scaling model requires the attainment of a specified value for the Weibull stress to trigger cleavage fracture in different specimens even though *J*-values may differ markedly. Here, we predict the distribution of cleavage fracture values for the deep crack SE(B) specimens ($a/W = 0.5$) using the distribution of measured fracture toughness for the precracked Charpy (PCVN) configuration.

Figures 4(a-b) show the computed evolution of σ_w with increased levels of loading, as characterized by *J*, for the deep crack SE(B) specimen and PCVN configuration using the calibrated *m*-values displayed previously in Table 1. Here, we direct attention to the evolution of σ_w *vs.* J derived from using $\gamma = 0$ (no plastic strain correction) and the plastic strain modified Beremin model (Eq. (5) previously described). In each plot, the correction $J_0^{PCVN_{a/W=0.5}} \rightarrow J_0^{SE(B)_{a/W=0.5}}$ defines the *predicted* J_0-value for the deep crack SE(B) specimen at $T = -80°C$ which then enables estimating the reference temperature, T_0, for the tested pressure vessel steel. Table 2 summarizes the *predicted* J_0-values and the estimated T_0 for all different forms of σ_w adopted in the present work.

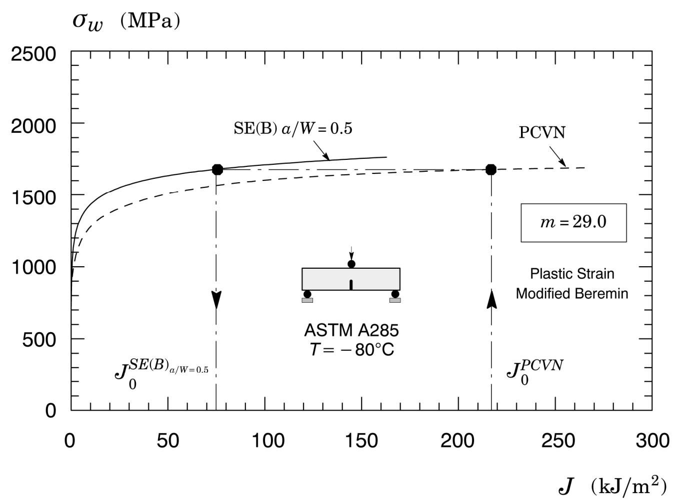
The sensitivity of J_0-predictions on the adopted formulation for σ_w is evident in these results which also strongly impacts estimates of T_0. The standard definition of σ_w described by previous Eq. (3), which is essentially the original Beremin model, provides a conservative estimate of T_0. In contrast, adoption of the linear plastic correction overpredicts the J_0-value for the deep crack SE(B) specimen and, consequently, the reference temperature. However, use of the plastic strain modified Beremin models yields a T_0 estimate which is in very good agreement with the corresponding estimate derived from the master curve analysis based on toughness values for the 1-T, deep crack SE(B) specimen with $a/W = 0.5$.

6. Concluding Remarks

This study describes a probabilistic framework based on the Weibull stress model to predict the effects of constraint loss on macroscopic measures of cleavage fracture toughness in the ductile-to-brittle transition region. A central objective is to determine the indexing temperature T_0 based on the Master Curve methodology from PCVN specimens. An additional feature of the proposed approach also includes the effect of near-tip plastic strain on cleavage microcracking which impacts directly the magnitude of the Weibull stress and, consequently, the toughness scaling curves. While the correction term included into the Weibull stress assumes an *ad-hoc* linear dependence of microcrack density on plastic strain, our exploratory analyses demonstrate the effectiveness of the Weibull stress model to provide estimates for the reference temperature, T_0, from small fracture specimens which are in good agreement with the corresponding estimates derived from testing of much larger crack configurations.



(a)



(b)

Figure 4. Weibull stress trajectories with increased levels of J for the deep crack SE(B) and PCVN specimens: (a) Standard Beremin model; (b) Plastic strain modified Beremin model.

Table 2. Estimates of J_0 and T_0 derived from different forms of the Weibull stress model

Weibull Stress Model	$\boldsymbol{J_0}$ (kJ/m^2)	$\boldsymbol{T_0}$ (∘C)
Standard Beremin ($\gamma = 0$ with no plastic strain correction)	54.1	-82.0
Generalized Weibull Stress with $\gamma = 1$ and $\beta = 0$ (linear correction)	100.8	-103.6
Generalized Weibull Stress with $\gamma = 1/2$ and $\beta = 0$ (square root correction)	137.6	-113.7
Plastic Strain Modified Beremin Model	74.1	-93.2

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