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# A local approach incorporating the measured statistics of microcracks to assess the temperature dependence of cleavage fracture for a reactor pressure vessel steel

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## Abstract

This work describes a local approach to cleavage fracture (LAF) incorporating the statistics of microcracks to characterize the cleavage fracture toughness distribution in structural steels. Fracture toughness testing conducted on standard compact tension C(T) specimens for a 22NiMoCr37 pressure vessel steel provides the cleavage fracture resistance data needed to determine the measured toughness distribution. Metallographic examination of etched surfaces for the tested steel also provides the distribution of carbides, which are assumed as the Griffith fracture-initiating particles, dispersed in the material from which the cleavage fracture toughness distribution is predicted. Overall, the analyses conducted in the present work show that LAFs incorporating the statistics of microcracks are a viable engineering procedure to describe the dependence of fracture toughness on temperature in the DBT region for ferritic steels.

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## 1. Introduction

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. 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, there has been renewed interest in developing more rational micromechanics-based methodologies for cleavage fracture assessments that have a direct bearing on accurate predictions of toughness measures across different crack configurations and loading modes. Here, attention has been primarily focused on probabilistic models

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incorporating weakest link statistics, most often referred to as local approaches to fracture (LAFs) (Beremin, 1983; Mudry, 1987; Pineau, 2006; Ruggieri and Dodds, 2018), 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 (1983) provided the impetus for 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 ( $\sigma_w$ ) as a probabilistic fracture parameter directly connected to the statistics of microcracks (weakest link philosophy). A key feature of this methodology is that  $\sigma_w$  incorporates both the effects of the near-tip stressed volume and the potentially strong variations 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 (Ruggieri and Dodds, 1996; Ruggieri, 2001; Ruggieri and Dodds, 2015; Ruggieri et al., 2015) by adopting the simple axiom that unstable crack propagation (cleavage) occurs at a critical value of the Weibull stress,  $\sigma_{w,c}$ .

However, while LAF methodologies represent a major advancement in current fracture assessment procedures to analyze the significance of defects and material degradation, difficulties still persist in engineering applications of the probabilistic model based on the Weibull stress concept that can have important implications for more accurate structural integrity assessments. Specifically, a major point of concern lies in the rather strong sensitivity of fracture predictions to the calibrated Weibull modulus, which is most often obtained based on limited experimental data (Ruggieri and Dodds, 2018) - typical values for parameter  $m$  range from 10 to 20 for structural ferritic materials, including common pressure vessel steels. Here, since  $\sigma_w$  scales with  $\int \sigma_1^m$  performed over the near-tip fracture process zone, larger  $m$ -values assign a greater weight factor to stresses at locations very near the crack front but, at the same time, reducing the potential contributions of near-tip material volume on the fracture probability - see full details in Ruggieri and Dodds (R&D) (2018). Hence, the resulting analysis based on the interpretation of  $\sigma_w$  as a macroscopic crack driving force may not uncover the controlling microfeatures for cleavage fracture, such as the actual fraction of eligible Griffith-like microcracks nucleated from the brittle particles effectively controlling cleavage fracture, thereby making the Weibull stress methodology insufficiently robust to serve as a more rigorous framework for cleavage fracture assessments.

Motivated by these observations, this exploratory work describes a local approach to cleavage fracture incorporating the measured statistics of microcracks to characterize the cleavage fracture toughness distribution in structural steels. One purpose of this study is to explore a theoretical framework consistent with what exists for probabilistic modeling of cleavage fracture to develop a failure probability model derived entirely from the measured carbide distribution dispersed into the ferritic matrix. Another is to explore application of the probabilistic model to describe the temperature dependence of  $J_c$ -values in the ductile-to-brittle (DBT) region for a nuclear pressure vessel steel. Fracture toughness testing conducted on standard compact tension C(T) specimens for a 22NiMoCr37 pressure vessel steel, known as the “Euro” Material A, provides the cleavage fracture resistance data needed to determine the experimentally measured  $J_c$ -distribution. Metallographic examination of etched surfaces for the Euro A steel also provides the distribution of carbides, which are assumed as the Griffith fracture-initiating particles, dispersed in the material from which the cleavage fracture toughness distribution is predicted. Overall, the analyses conducted in the present work show that LAFs incorporating the statistics of microcracks are a viable engineering procedure to describe the dependence of fracture toughness on temperature in the DBT region for ferritic steels.

## 2. Cleavage Fracture Modeling Incorporating the Microcrack Distribution

Early progress in understanding the mechanisms of brittle fracture in mild steels was achieved by means of detailed metallographic observations of cleavage microcracks. A number of works, including that of Low (1953), Owen and Averbach (1958), McMahon and Cohen (1965) and Smith (1968), revealed the formation of Griffith-like microcracks (Griffith, 1921) after the onset of yielding and localized plasticity primarily by the cracking of carbides along grain boundaries. Further analyses of the microstructural features, as those represented by the early works of Curry and

Knott (1978; 1979), reveal that only *eligible* particles, which are associated with large dislocation pile-ups acting as suitable stress raisers and favorable orientation, can produce Griffith-like microcracks. 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 (Hahn, 1984). The connection between fracture resistance and microstructure can then be made by rationalizing the interrelation between microcrack nucleation and unstable propagation in a multi-step process: a) fracture of a carbide particle assisted by plastic deformation of the surrounding matrix nucleates a Griffith-like microcrack; b) the nucleated microcrack advances rapidly into the interior of the ferrite grain until it reaches a grain boundary and c) fracture occurs when the microcrack is not arrested at a grain boundary barrier and thus propagates unstably. In terms of the Griffith cleavage criterion (Griffith, 1921), the last condition means that the Griffith fracture energy to propagate the microcrack is larger than the specific surface energy of the grain boundary (Hahn, 1984).

Development of the probabilistic formulation incorporating the distribution of microcracks begins with consideration of the near-tip fracture process zone (FPZ) ahead of a stationary macroscopic crack lying in a material containing randomly oriented microcracks, uniformly distributed in location. Further consider that the near-tip FPZ is idealized as consisting of a large number of statistically independent, uniformly stressed, small volume elements, denoted  $\delta V$ , and which are subjected to the principal stress,  $\sigma_1$ , and associated effective plastic strain,  $\epsilon_p$ , as illustrated in Fig. 1(a). Now let  $N_c$  be the number of microcracks nucleated from fractured carbides in the small volume,  $\delta V$ , given by

$$N_c = \Psi_c \rho_d \delta V \quad (1)$$

where  $\rho_d$  is the (average) density of carbides in the FPZ material and  $\Psi_c$  represents the fraction of fractured carbides which are assumed as the Griffith-like microcracks that are eligible to propagate unstably with  $0 \leq \Psi_c \leq 1$ .

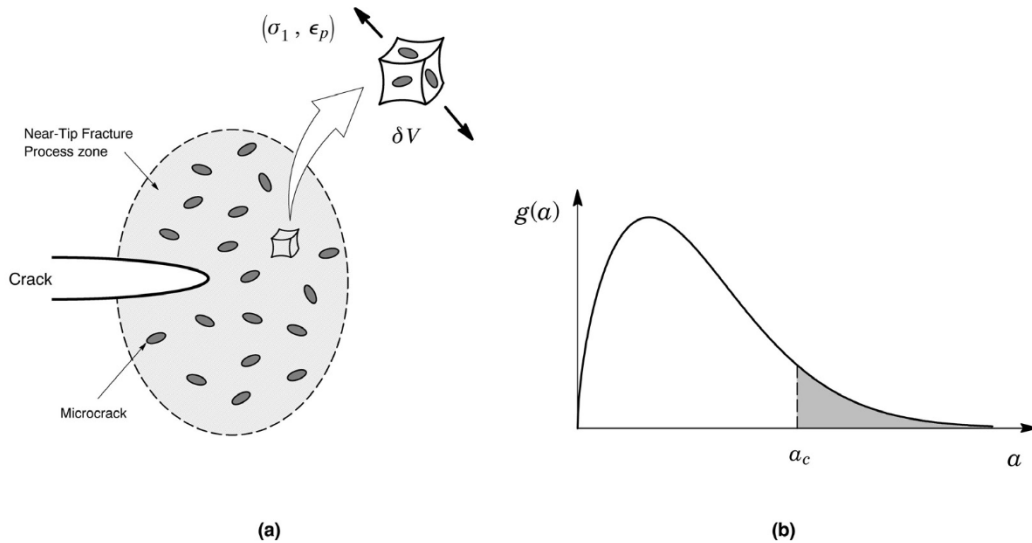


Fig. 1. (a) Near-tip fracture process zone ahead a macroscopic crack containing randomly distributed flaws. b) Schematic of probability density function (*pdf*) to describe the microcrack size distribution.

The specific micromechanism of transgranular cleavage allows assuming that failure of each small volume element occurs when the size of a random microcrack contained in  $\delta V$  exceeds a critical size, *i.e.*,  $a \geq a_c$ . Thus, using weakest link arguments in connection with the assumption that cleavage fracture is governed by the failure of a small volume element,  $\delta V$ , the failure probability for the cracked body,  $P_f$ , is expressed as

$$P_f = 1 - \exp \left\{ \int_{V_{FPZ}} \ln \left[ \int_0^{a_c} g(a) da \right]^{N_c} dV_{FPZ} \right\} \quad (2)$$



in which  $g(a)da$  defines the probability of finding a microcrack having size between  $a$  and  $a + da$  in the small volume as depicted in Fig. 1(b), and it is also understood that the integral is performed over the volume of the near-tip fracture process zone,  $V_{FPZ}$ .

In the above, the critical microcrack size,  $a_c$ , follows from a modified form of the Griffith criterion (Anderson, 2005) expressed as

$$a_c = \frac{2E\gamma_f}{\pi(1-\nu^2)\sigma_1^2} \quad (3)$$

where  $E$  is the Young's modulus,  $\nu$  denotes the Poisson's ratio and  $\sigma_1$  represents the maximum principal stress acting normal to the microcrack plane. Here,  $\gamma_f = \gamma_s + \gamma_p$  defines the effective fracture energy to propagate the microcrack in which  $\gamma_s$  is the (elastic) surface energy and  $\gamma_p$  is the temperature dependent, plastic work per unit area of surface created.

### 3. Experimental Fracture Toughness Data

Extensive fracture toughness tests were performed on a nuclear reactor pressure vessel (RPV) class steel DIN 22NiMoCr37 similar to ASTM A508 Cl.3 steel and widely referred to as “Euro” Material A. Conducted as part of the “Measurement and Testing Programme of the European Commission”, the testing program focused primarily on developing an experimental fracture toughness data base for validation of the Master Curve methodology, including an experimental investigation of specimen geometry and temperature effects on fracture toughness in ferritic materials. Heerens and Hellmann (H&H) (2002) provide a detailed description of the Euro fracture toughness dataset. Here, we limit attention to selected fracture toughness distributions measured at four test temperatures:  $T = -154^\circ\text{C}$ ,  $-110^\circ\text{C}$ ,  $-91^\circ\text{C}$  and  $-60^\circ\text{C}$ . H&H (2002) also provide the mechanical properties for the tested material for these test temperatures.

The cumulative Weibull distributions of the measured  $J_c$ -values are displayed in Fig. 2 in which the solid symbols in the plots represent the experimentally measured fracture toughness. The fracture toughness tests were performed on conventional, plane-sided compact tension C(T) specimens with  $a/W \approx 0.55$ . The fracture mechanics tests include: (1) 0.5T C(T) specimens ( $B = 12.5$  mm) tested at  $T = -110^\circ\text{C}$ ; (2) 1T C(T) specimens ( $B = 25$  mm) tested at  $T = -154^\circ\text{C}$ ,  $-91^\circ\text{C}$  and  $-60^\circ\text{C}$ . Here,  $a$  is the crack size and  $W$  denotes the specimen width. In this plot, the cumulative probability,  $F(J_c)$ , is derived by simply ranking the  $J_c$ -values in ascending order and using the median rank position defined in terms of  $F(J_c) = (k - 0.3)/(N + 0.4)$ , where  $k$  denotes the rank number and  $N$  defines the total number of experimental toughness values. The fitting curves to the experimental data shown in this figure describe the three-parameter Weibull distribution for  $J_c$ -values with a fixed value of  $\alpha = 2$  as the Weibull modulus and a threshold  $J$ -value corresponding to a  $K_{min} = 20$  MPa  $\sqrt{\text{m}}$ .

### 4. Finite Element Procedures

Nonlinear finite element analyses are performed on detailed 3-D models of the tested C(T) specimens with  $a/W \approx 0.55$  described previously. Figure 3 shows the finite element model utilized in the analyses of the 1T C(T) specimen with  $B = 25$  mm. With minor differences, the numerical model for the 0.5T C(T) specimen with  $B = 12.5$  mm has very similar features. 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 having radius  $\rho_0 = 0.0025$  mm. Symmetry conditions enable analyses using one-quarter of the 3-D models with appropriate constraints imposed on the symmetry planes. The quarter-symmetric, 3-D model for this specimen has 25 variable thickness layers and approximately 40,000 nodes and 36,000 8-node, 3-D elements.

The finite element code WARP3D (Healy et al., 2014) provides the numerical solutions for the 3-D analyses reported here. The finite element analyses utilize an elastic-plastic constitutive model with flow theory and conventional Mises plasticity in large geometry change (LGC) setting incorporating a simple power-hardening model to characterize the uniaxial true stress vs. logarithmic strain with the hardening exponent estimated from the flow properties given by H&H (2002).

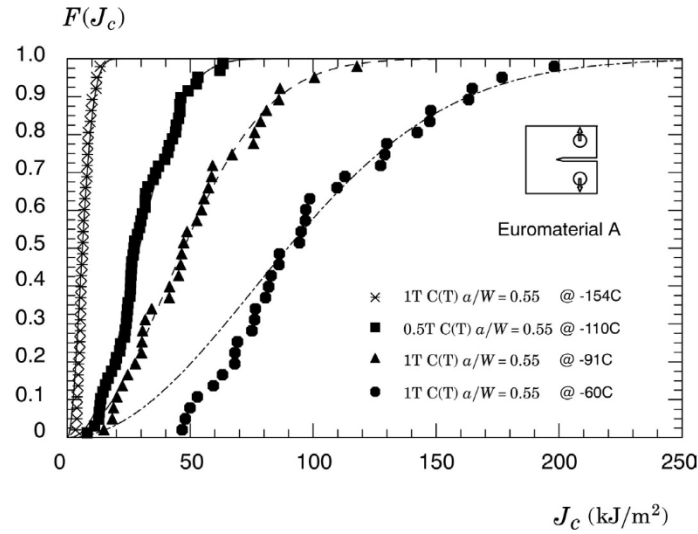


Fig. 2. Cumulative Weibull distribution of the measured  $J_c$ -values for the “Euro” Material A at test temperatures:  $T = -154^\circ\text{C}$ ,  $-110^\circ\text{C}$ ,  $-91^\circ\text{C}$  and  $-60^\circ\text{C}$ .

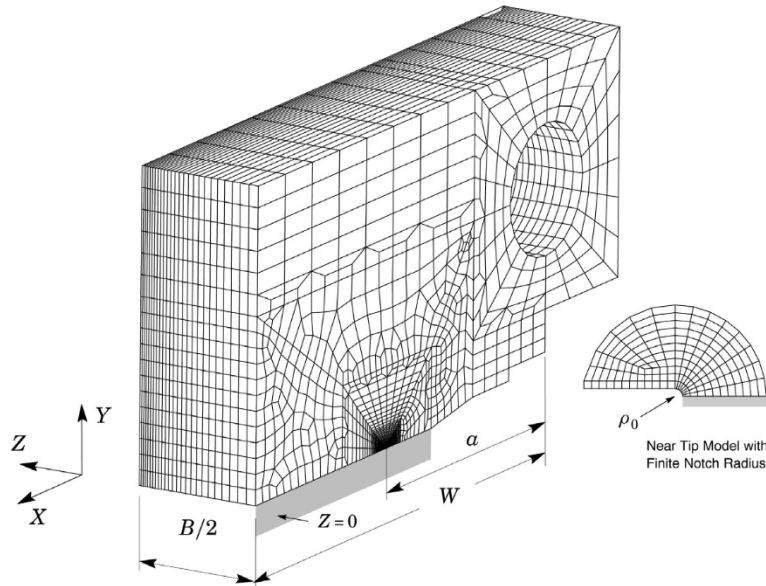


Fig. 3. 3-D FE model of the 1T C(T) specimen with  $a/W \approx 0.55$  and  $B = 25$  mm.

## 5. Prediction of Temperature Effects on Fracture Toughness

### 5.1. Model Calibration

Calibration of the probabilistic model follows from matching the predicted toughness distribution with the experimentally measured  $J_c$ -values for the 1T C(T) specimens tested at  $T = -154^\circ\text{C}$ . This specimen arguably provides the lowest levels of crack-tip plastic deformation and thus minimizes the dependence of the critical microcrack size,  $a_c$ , on the temperature dependent, plastic work  $\gamma_p$ . Moreover, based on the carbide size measurements for the Euro

Material A conducted by Ortner et al. (2005), we adopt a two-parameter Weibull distribution to describe the *pdf* for the carbide size,  $g(a)$ , appearing in Eq. 2 and expressed as

$$g(a) = \frac{\alpha_c}{\beta_c} \left( \frac{a}{\beta_c} \right)^{\alpha_c - 1} \exp \left[ - \left( \frac{a}{\beta_c} \right)^{\alpha_c} \right] \quad (4)$$

in which a fitting procedure yields  $\alpha_c = 1.996$  and  $\beta_c = 7.876 \cdot 10^{-5}$  mm. Figure 4 shows the histogram of the particle size distribution corresponding to an average density of carbides,  $\rho_d = 7.6 \cdot 10^8 \text{ mm}^{-3}$  measured by Ortner et al. (2005) which also includes the fitted two-parameter Weibull distribution.

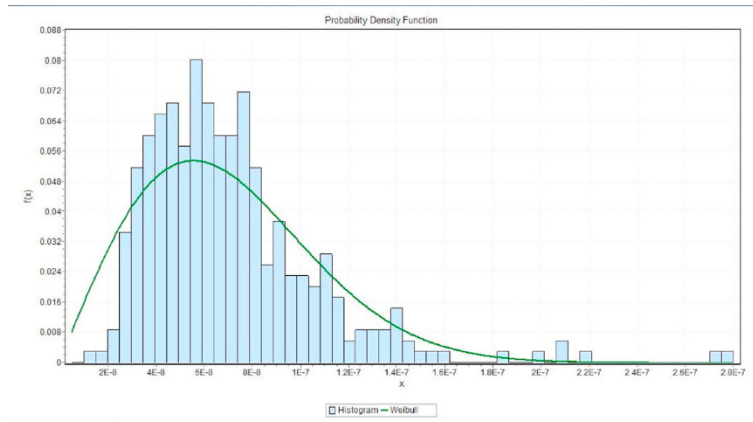


Fig. 4. Histogram of the particle size distribution measured by Ortner et al. (2005), including the fitted two-parameter Weibull *pdf*.

## 5.2. Fracture Toughness Predictions

The procedure used here to predict the effects of temperature on the experimental cleavage fracture toughness data of the tested nuclear pressure vessel steel derives from solving Eq. (2) at each load step once all parameters are determined. Figure 5 displays the predicted toughness distribution for the 1T C(T) specimen tested at  $T = -154^\circ\text{C}$  with the fraction of fractured carbides,  $\Psi_c$ , described by a Pareto type function (Arnold, 2015) in the form

$$\Psi_c = 1 - \left( \frac{\epsilon_{ys}}{\epsilon_p} \right)^2 \quad (5)$$

where  $\epsilon_{ys} = \sigma_{ys}/E$  with  $\sigma_{ys}$  representing the yield stress at the test temperature. For the Euro Material A at  $T = -154^\circ\text{C}$ , adopting an effective fracture energy of  $\gamma_f = 6 \text{ J/m}^2$  provides good agreement between the measured and predicted toughness distributions.

To arrive at the toughness distributions for other test temperatures, we adopt the following procedure. First, we determine the predicted toughness distribution at  $T = -60^\circ\text{C}$  with a calibrated value of  $\gamma_f = 7.3 \text{ J/m}^2$  which provides the best fit to the measured distribution of  $J_c$ -values as illustrated in Fig. 6. Next, by adopting the surface energy of iron as  $\gamma_s = 2 \text{ J/m}^2$  and following similar procedure outlined in Wallin et al. (1984), we determine the temperature dependence of  $\gamma_p$  and, consequently,  $\gamma_f$  in the form

$$\gamma_f = 2 + 6.35 \cdot \exp(0.003T) \quad (6)$$

where  $T$  is the test temperature in degrees Celsius. Figure 6 also shows the predicted toughness distributions for the C(T) specimens tested at  $T = -110^\circ\text{C}$  and  $-91^\circ\text{C}$  in which general good agreement with the measured data is observed.

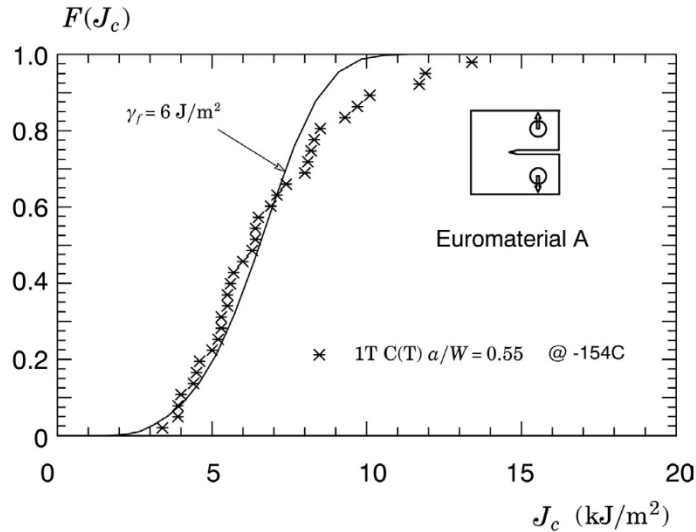


Fig. 5. Predicted toughness distribution for the 1T C(T) specimen tested at  $T = -154^{\circ}\text{C}$  with  $\gamma_f = 6 \text{ J/m}^2$ .

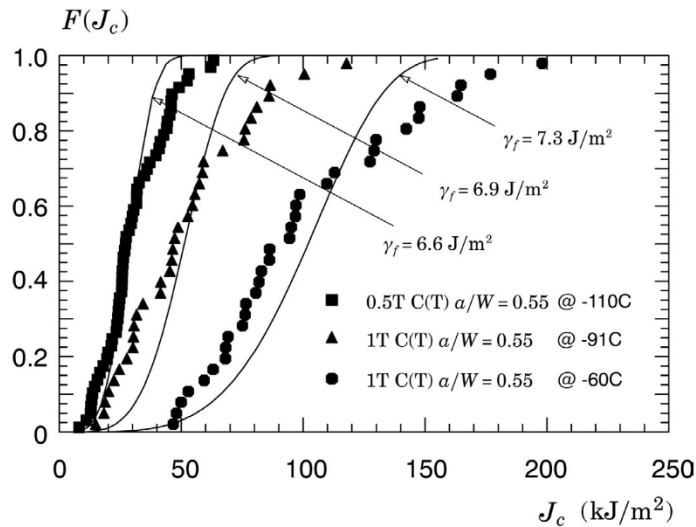


Fig. 6. Fitted toughness distribution for the C(T) specimen tested at  $T = -110^{\circ}\text{C}$  and  $-91^{\circ}\text{C}$  with varying values for the effective fracture energy,  $\gamma_f$ .

## 6. Concluding Remarks

This work describes an exploratory application of a local approach to cleavage fracture incorporating the measured distribution of carbides and brittle particles. The analyses conducted in the present work show that predictions of the temperature dependence of  $J_c$ -values are in good agreement with the measured toughness distributions. However, calibration of the key parameters controlling cleavage fracture still remains rather complex for robust applications of the probabilistic model in routine structural integrity assessments. In particular, a clear and simple estimation procedure for the temperature dependent, plastic work parameter,  $\gamma_f$ , is still considered an open issue and work along this line of investigation is in progress. Overall, the present analyses show that LAFs incorporating the statistics of microcracks appear a viable engineering procedure to describe the dependence of fracture toughness on temperature in the DBT region for ferritic steels.

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