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Fracture Toughness of Ferritic Steels in the Ductile-to-Brittle Transition Region

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Abstract

Ferritic steels, as other materials, have different failure modes depending on the temperature. At elevated temperatures, they behave as ductile materials, while at low temperatures they are brittle. There is an intermediate temperature region where these alloys have a failure mode resulting from the competition between cleavage and ductile mechanisms. This region is known as the ductile-to-brittle transition zone. The characterization of fracture resistance of ferritic steels in the ductile-to-brittle transition region is problematic due to scatter in results, as well as size and temperature dependences. American Society for Testing and Materials (ASTM) has standardized the determination of a temperature reference (T_0) for the fracture toughness characterization of ferritic steels in this region. This chapter presents the evolution of the statistical treatment of fracture toughness data until the present, including some comments on T_0 determination, and some aspects that require a deeper analysis.

Keywords: ductile-to-brittle, fracture toughness, ferritic steels, weakest link, master

1. Introduction

curve

The so-called ferritic steels are, as defined in American Society for Testing and Materials (ASTM) E1921-2015a^{ε 1} [1], "typically carbon, low-alloy, and higher alloy grades. Typical microstructures are bainite, tempered bainite, tempered martensite, and ferrite and pearlite. All ferritic steels have body centered cubic crystal structures that display ductile-to-cleavage transition temperature fracture toughness characteristics."



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Ferritic steels, as other materials, have different failure modes depending on the temperature. At elevated temperatures, they behave as ductile materials, while at low temperatures they are brittle. There is an intermediate temperature region where these alloys have a failure mode resulting from the competition between cleavage and ductile mechanisms. This region is known as the ductile-to-brittle transition zone, where fracture toughness decreases with decreasing temperatures. **Figure 1** shows the fracture behavior of different materials with temperature, including some that don't have a transition zone.



Figure 1. Fracture behavior of different materials as a function of temperature.

The characterization of fracture resistance of ferritic steels in this region is problematic due to scatter in results, as well as size and temperature dependences [2–9].

Size effects imply decreasing of the median value of fracture toughness and a larger scatter in small specimen than in larger ones. **Figure 2** describes schematically the failure probability density functions for a material in equal conditions but with two different sizes (thicknesses B_1 and B_N), using *Jc* as the fracture toughness parameter.



Figure 2. Weibull probability density function for two specimen sizes.

Originally, there were two explanations to the size effect. One was based on constraint effects, while the other made use of statistical weakest link concepts to explain the probability to find a cleavage initiator site at the crack front.

1.1. Constraint theory

This theory is based on the hypothesis that specimens with larger thickness present larger constraint than thinner specimens and that the average fracture toughness will be smaller for larger specimens than for smaller ones [10]. But this theory fails to explain the differences in scatter for different sizes.

1.2. Statistical theory

According to this theory, there are small areas of low toughness or weak links (possible initiators of cleavage) randomly distributed in the crack front, so that the brittle fracture would be a statistical event (Landes and Schaffer [11], Landes and McCabe [12]). The cleavage fracture is a local fracture process controlled by a critical stress, and it will occur when the critical stress is reached in one of these weak links. The load required to produce the fracture will depend upon the location of the weak link and its critical stress.

In addition to the scatter that occurs in the transition region, the weakest link model also explains the effect of specimen size, since an increase in the length of the crack front enlarges the highly stressed volume of material at the tip of the crack, also increasing the likelihood to find a weak link.

Based mainly on the works of Wallin [13–16], with the master curve (MC) methodology, the ASTM has standardized the determination of a temperature reference (T_0) for the fracture toughness characterization of ferritic steels in this region.

This chapter presents the evolution of the statistical treatment of fracture toughness data, including some comments on T_0 determination, and some aspects that require a deeper analysis.

2. Evolution of the statistical-based theory

2.1. Weakest link original proposal

Waloddi Weibull [17] proposed a probability distribution function (later called Weibull distribution). The probability of choosing an individual with a value X less than a given value x is given by Eq. (1):

$$P(X \le x) = P(x) = 1 - \exp(-\varphi(x)) \tag{1}$$

The function $\varphi(x)$ can have any expression, although the simplest one is

$$\varphi(x) = \left(\frac{x-a}{b}\right)^c \tag{2}$$

where

a: threshold parameter

c: shape parameter or Weibull slope

b: scale parameter

Equation (3) results from replacing $\varphi(x)$ of Eq. (1) with Eq. (2):

$$P(x) = 1 - \exp\left(-\left(\frac{x-a}{b}\right)^c\right)$$
(3)

The probability density function is

$$f(x) = \frac{dP}{dx} \tag{4}$$

If we have a chain with *N* links, with each of them having a probability of failure *P*, the chain will fail when the weakest link fails, so the "non-failure" probability of the chain is

$$(1 - P_N) = (1 - P)^N$$
(5)

Then, the chain failure probability is

$$P_{N}(x) = 1 - \exp(-N\varphi(x))$$
(6)

2.2. Landes proposal

In 1980, Landes and Shaffer [11] proposed that the cleavage fracture toughness of a metallic specimen is controlled by the point of minimum toughness (weakest link) at the crack front. According to these authors, it would be possible to predict the fracture toughness of large structures or specimens by testing small specimens. Using a two-parameter Weibull (2P-W) distribution, adapting the names of the variables and parameters, they proposed Eq. (7) as the failure probability for a specimen thickness B:

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$$P = 1 - \exp\left(-\left(\frac{Jc}{J_0}\right)^b\right) \tag{7}$$

The non-failure probability is

$$1 - P = \exp\left(-\left(\frac{Jc}{J_0}\right)^b\right)$$
(8)

For a thickness B_N = N.B:

$$(1-P_N) = (1-P)^N = \exp\left(-N\left(\frac{Jc}{J_0}\right)^b\right)$$
(9)

The failure probability for a B_N thickness results

$$P_{N} = 1 - \exp\left(-N\left(\frac{Jc}{J_{0}}\right)^{b}\right)$$
(10)

The problem with this distribution is that the mean Jc value of the sample, Eq. (11), tends to zero when N tends to infinity (very large thicknesses), which is physically impossible since every material has a minimum value of toughness:

$$\overline{J_c} = \frac{J_0}{N^{\frac{1}{b}}}$$
(11)

In order to solve this problem, Landes and McCabe [12] proposed to use a three-parameter Weibull function (3P-W), where the third parameter J_{min} corresponds to a threshold parameter. **Figure 2** shows schematically the probability density functions derived from the probability distribution given by Eq. (12), where the same threshold for both distributions can be observed for different sizes. If the effect of size is incorporated, Eq. (13) would be applied but considering *b* and J_0 parameters from the distribution for *B* size. In this case, the probability density functions observed in **Figure 2** would be coincident.

For thickness *B*:

$$P = 1 - \exp\left(-\left(\frac{Jc - J_{\min}}{J_0 - J_{\min}}\right)^b\right)$$
(12)

For thickness
$$B_N = N.B$$
:

$$P = 1 - \exp\left(-N\left(\frac{Jc - J_{\min}}{J_0 - J_{\min}}\right)^b\right)$$
(13)

It should be highlighted that Landes and McCabe [12] found that the weakest link theory (expressed by a 3P-W function) described well the thickness effect in the fracture toughness observed in the ductile-to-brittle transition region. But this theory of weakest link does not have a theoretical basis to justify the relationship between the weakest link and the function of Weibull distribution, but it was stated that the latter is adjusted to the experimental data.

2.3. Kim Wallin proposal

Wallin [13–16] assumed that the crack-front material presents a random distribution of potential cleavage initiators. The cumulative probability distribution for a single critical site is a complex function that depends, among other things, on the size distribution of the initiators, stress, strain, temperature, loading rate, etc. It is considered that the shape and origin of the initiators distribution is not important for the case of sharp cracks, and no global interaction between initiators exists. It is considered that there is no interaction between initiators on a global scale. It may happen that there is a cluster of initiators to start the macroscopic fracture, and in this case the cluster is treated as a single site.

By means of theoretical assumptions of the probability distribution of volume elements near the crack tip and complex mathematical deductions, Wallin obtained the following expression for the probability of failure:

$$P = 1 - \exp\left[-\text{constant} \cdot \mathbf{B} \cdot K_I^4\right]$$
(14)

Note that the shape parameter is fixed and equal to 4. The theoretical assumptions of Wallin, although different to those raised originally by Weibull, are also based on a weakest link failure mechanism.

Taking into account the existence of a minimum value of toughness, Eq. (14) is modified introducing a threshold parameter, and taking into account a conditional crack propagation criterion results in Eq. (15):

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$$P = 1 - \exp\left[-\text{constant} \cdot \mathbf{B} \cdot \left(K_I - K_{\min}\right)^4\right]$$
(15)

Equation (15) is expressed in the form of Eq. (16):

$$P = 1 - \exp\left(-\frac{B}{B_0} \left(\frac{K_{Jc} - K_{\min}}{K_0 - K_{\min}}\right)^4\right)$$
(16)

where K_0 and B_0 are normalization constants.

Wallin [18] concluded that, despite the fact that K_{\min} depends on the temperature and material, the value that fits the data better using small sample sizes is 20 MPa.m^{1/2}.

2.4. Other proposals

According to Anderson et al. [19], the probability of failure based on the weakest link model corresponds to a 2P-W distribution of the type

$$P = 1 - \exp\left[-\frac{B}{B_0}\left(\frac{J_c}{J_0}\right)^2\right]$$
(17)

or, in terms of *K*:

$$P = 1 - \exp\left(-\frac{B}{B_0} \left(\frac{K_{Jc}}{K_0}\right)^4\right)$$
(18)

Regarding the type of distribution, 2P-W or 3P-W parameters, the use of both distributions is used in the classical literature [20–22]. The trend is to use a distribution with fixed parameters, which reduces the amount of specimens required to obtain the statistical distribution in a set of data, as would only have to determine a single parameter of the distribution (Eqs. (19) and (20)):

$$P = 1 - \exp\left[-\left(\frac{J_C}{J_0}\right)^2\right]$$
(19)

$$P = 1 - \exp\left(-\left(\frac{K_{Jc} - 20}{K_0 - 20}\right)^4\right)$$
(20)

Nowadays, 3P-W is well accepted in terms of *K* given by Eq. (20), due to the small sample size necessary for the estimation of K_0 . According to McCabe [21], such a practice would only be suitable for establishing trends in mean toughness, however, because the tails of the fitted distribution curves would be quite unreliable and not usable to estimate lower-bound values.

3. Master curve

Kim Wallin [16] proposed that most ferritic steels tend to conform to one universal curve of median fracture toughness versus temperature for 1-inch thick specimens (Eq. (21), **Figure 3**). The temperature dependence of the 1 T-C(*T*) median fracture toughness is based on an empirical equation calibrated at the T_0 temperature that corresponds to a K_{Jc} (med) = 100 MPa.m^{0.5} (Eq. (21)). *T* refers to the test temperature:

$$K_{Jc(med)} = 30 + 70 \exp(0.019(T - T_0))$$
⁽²¹⁾

This curve, named MC, was standardized in 1997 by ASTM, after several decades of scientific investigations, with the effort of researchers all over the world and the realization of some round-robin projects. The last version of the standard is ASTM E1921-15a^{ϵ 1} [1].



Figure 3. Master Curve.

The reference temperature (T_0) must be known to place the curve in the temperature axis and then have the fracture toughness characterization of ferritic steels in this region. The standardized procedure includes a size conversion equation for those situations where different specimen sizes are used, and some instructions for censoring data for excessive plasticity and ductile crack growth prior to fracture and for loss of constraint.

As the standard makes use of linear elastic fracture mechanics and the measurement of the fracture toughness is made by means of the elastic plastic *Jc* parameter, their values have to be converted to K_{Jc} equivalent values by means of Eq. (22), where *E* and v are the Young and the Poisson modulus, respectively.

$$K_{J_C} = \sqrt{\frac{J_C \cdot E}{1 - v^2}} \tag{22}$$

The MC concept is based on a 3P-W distribution with shape parameter equal to 4 and threshold value equal to 20 MPa.m^{0.5}, for compact specimens of 1-inch size (Eq. (20)). In this way, only K_0 must be estimated.

ASTM E1921-15a^{ϵ 1} [1] sets up a procedure for K_0 determination. It includes the conversion of the K_{Jc} values obtained for *B* thickness specimens to 1-inch size equivalent ($K_{Jc(1T)}$) by means of Eq. (23), as well as specifications for data censoring:

$$K_{J_{c(1T)}} = 20 + (K_{JC} - 20)B^{1/4}$$
(23)

This standard imposes two limits for K_{Jc} values: the first one is given by the condition of a high crack-front constraint at fracture (Eq. (24)):



The second limit states that K_{Jc} values also shall be regarded as invalid for tests that terminate in cleavage after more than $0.05(W-a_0)$ or 1 mm (0.040 in.), whichever is smaller, of slow-stable crack growth.

The standardized procedure includes some instructions for censoring data for excessive plasticity and ductile crack growth prior to fracture and for loss of constraint.

 K_0 is calculated by means of Eq. (25):

$$K_{0} = \left[\sum_{i=1}^{N} \frac{\left(K_{J_{c}(i)} - 20\right)^{4}}{r}\right]^{\frac{1}{4}} + 20$$
(25)

 $K_{Jc(i)}$ corresponds to the individual K_{Jc} (originally 1 inch or converted to 1 inch equivalent), *r* is the quantity of non-censored tests, and *N* is the total number of tests.

The ASTM E1921-15a^{ϵ 1} [1] standard also allows the T_0 determination for testing speeds other than static test and for different specimen configurations or geometries, besides the fact that single or multiple temperature tests are considered.

Prior to the MC, ASME Boiler and Pressure Vessel Code already established the lower-bound K_{IC} and K_{Ia} curves for the characterization of ferritic pressure vessel steels [23]. The reference temperature was RT_{NDT} instead of T_0 (**Figure 4**). The implementation of the MC has been a huge advance in the need to have adequate tools for treating the complexities related to temperature, size, and scatter in the ductile-to-brittle transition region for ferritic steels.



4. Some aspects on the statistical data fitting

The relationship between the parameters *K* and *J* given by Eq. (22) would lead one to believe that the Weibull slope in terms of *K* (b_K) is twice the slope (b_I) when *J* data are used.

It would appear correct to think that $b_K = 2b_J$, so if it is accepted that $b_K = 4$, the b_J value would be 2. But this is only valid when working with two-parameter distributions, without a threshold parameter.

An analysis about the relationship between Weibull distributions expressed in terms of *J* and *K* was presented in reference [7]. It was shown that if the J_c results follow a 3P-W, their equivalent K_{JC} values do not exactly fit a 3P-W function obtained by means of a simple transformation of the three parameters. Nevertheless, an approximated 3P-W function in *K* terms was proposed. It fits very well with the transformed values and their parameters are related to the ones expressed in *J* terms.

Equation (22) is applied to convert J_{min} and J_0 parameters, resulting in the new parameters of the *K* distribution from Eqs. (26) and (27):

$$K_{\min} = K_{J_{\min}} = \sqrt{\frac{EJ_{\min}}{(1 - v^2)}}$$
(26)

$$K_0 = K_{J_0} = \sqrt{\frac{EJ_0}{(1 - v^2)}}$$
(27)

The shape parameter b_K must be calculated by means of Eq. (28):

$$b_{K} = 2 \frac{K_{0}}{K_{0} + K_{\min}} b_{J} = \xi \ b_{J}$$
(28)

Figure 5 shows values of ξ as a function of different combinations of K_0 and K_{\min} . As already expressed, for the particular situation of a 2P-W, there is an exact equivalence between the distributions in terms of *J* and *K*, being the Weibull slope in terms of *K* twice the slope in terms of *J* (K_{\min} = 0).

Figure 6 shows an example where a dataset of *K* values, transformed from *Jc*, is fitted using Weibull-based statistical distributions. The differences among them are the way the three parameters were obtained and are as follows:

- parameters estimated from *K*_{*lc*} values converted from *Jc*,
- parameters calculated using Eqs. (26)-(28),
- parameters K_{\min} and K_0 obtained using Eqs. (26) and (27); $b_K = 2b_I$.

Clearly, the latter only coincides with the others in zone B, near a failure probability of P = 0.63. The first two distributions are quite similar for all the probability levels, including zone C (near the lower-bound zone) and for high probability levels (zone A).



Figure 5. Dependence of ξ with K_0 and K_{\min} .



Figure 6. Comparison of cumulative probabilities obtained considering different options.

5. Unresolved aspects on the transition

The MC is a methodology to deal with the calculation of K_{Jmean} in the transition region using small datasets. Despite the fact that it is a good response to an engineering problem, there are some aspects of the transition region that must be investigated.

5.1. The real transition region

Perez Ipiña et al. [5] presented a ductile-to-brittle region reinterpretation based on experimental evidence (**Figure 7**). They proposed not a single curve but the area involving the scatter band. This area is limited by two curves, one corresponding to the toughness lower bound (thickness independent, i.e., material property) and the other fitting to the upper limit of the scatter band (thickness dependent). In this way, the area is larger for smaller thickness than for larger ones. Note that the scatter in ductile mechanisms is much lower than in cleavage.



Figure 7. Ductile-to-brittle region scatter band for (a) small specimens and (b) large specimens.





Figure 8. (a) Subregion III and (b) subregion III' in the ductile-to-brittle transition curve.

I: All specimens fracture by cleavage without any stable crack growth.

II: Some specimens fracture by cleavage without any stable crack growth, while others fracture by cleavage after some amount of stable crack growth.

III: No cleavage without stable crack growth occurs. All the specimens fracture by cleavage after some amount of stable crack growth, or

III: some specimens fracture without stable crack growth, others with stable crack growth, and others reach the maximum load condition and do not present instability.

III or III' will be present depending on the crossing of curves J_{IC} with lower-bound cleavage and the crossing of J_{max} with upper-bound cleavage curves. When the intersection of J_{IC} with the cleavage lower-bound curves and the intersection of J_{max} with the cleavage upper-bound curves occur at the same temperature, there will be no region III nor III'.

IV: Some specimens fracture after some amount of stable crack growth, while others reach the maximum load condition and do not present instability.

For higher temperatures, no cleavage occurs and this behavior corresponds to the upper shelf.

Maximum load toughness is size dependent: small specimens present the P_{max} plateau close past the stable crack growth initiation, while large specimens require more stable crack growth to reach this plateau, giving them larger J_{max} than small specimens. Maximum load curves intersect the cleavage curves—the upper cleavage curve is also size dependent—at different temperatures for different sizes, **Figure 8**. Region IV widens and displaces toward higher temperatures as size increases, making the beginning of the upper shelf also size dependent, as stated by Wallin [24].

5.2. Stable crack growth and loss of constraint limitations

In subregions where some or all specimens present ductile growth of cracks (DCG), the probability of failure of a set of data is affected by this stable growth. It may also happen that conditions of maximum $J(J_{max})$ are violated for small specimens and the fracture toughness of these samples will increase as a consequence of a loss of constraint. **Figure 9** [20] shows schematically these two effects in the cumulative failure probability.

Consequently, the weakest link model, and the toughness prediction for different thicknesses, seems not to work well in the superior third of the transition region, where ductile crack growth and/or loss of constraint are present. There are therefore conditions that must be met for its implementation. There are various proposals or explanations in the literature of the area of validity of the model weakest link. Among these is the existence of a single initiator of cleavage site, and limitations in the stable growth of cracks prior to cleavage (would affect the in-plane constraint) and in the thickness of the sample (would affect the out-of-plane constraint). The MC, as mentioned before, introduces censoring under conditions of stable crack growth or loss of constraint. This censoring scheme, when applied to 3P-W, gives artificially increased slope values.



Figure 9. Effects of ductile tearing and decreasing constraint.

Some authors (Wallin [15] and McCabe et al. [22]) also stated that the model is not valid at temperatures corresponding to the lower shelf.

The use of small datasets does not allow a correct K_{\min} and b_K estimation. Berejnoi and Perez Ipiña [4] have shown that the threshold parameter K_{\min} and Weibull slope b_K are clearly dependent on temperature and different from the values of 20 MPa.m^{0.5} and 4, which are considered in the MC. This was found even for 1-inch size sets with all valid data. **Figure 10** shows the MC from the material of the Euro round-robin [25] obtained with 1-inch specimens, corresponding to a T_0 =-96°C. The values of K_{Jmean} obtained using MC methodology at different temperatures and sizes are also shown, being clearly different from the MC.



Figure 10. *K*_{med} versus *T* for different sizes and master curve according to ASTM E1921.

When only valid datasets of 1-inch size are considered [4], the values of K_0 and K_{med} obtained using a 3P-W distribution are in concordance with those obtained using ASTM E1921-15a^{ε1}[1], although b_k and K_{min} were different. The fixed values stated in ASTM standard could not be appropriated when a size conversion criterion and/or some censoring procedure are included.

Figure 11 corresponds to datasets from the Euro round-robin, tested at T = -60 °C using 2-inch specimens. This temperature is within the range of $T_0 + 50$ °C of the material. The original data were converted to a 1-inch equivalent size, by means of Eq. (22). This procedure was also applied considering the 3P-W distribution with $b_K = 4$ and $K_{\min} = 20$ (Eq. (20)).



Figure 11. Probability distributions for $T = -60^{\circ}$ C and 2*T* original dataset.

From **Figure 11**, it is seen that the conversion formula does not work properly, and it is not just as simple as using a factor *N* as the weakest link model states for converting toughness values, nor with 3P-W, nor with MC. The distributions (MC or 3P-W) do not fit the toughness values obtained experimentally using 1T size. Experimental converted-to-1T values (green circles in **Figure 11**) should be close to the original 1T values (black crosses).

6. Conclusions

The characterization of fracture resistance of ferritic steels in the ductile-to-brittle transition region is problematic due to scatter in results, as well as size and temperature dependences.

Originally, there were two explanations to the size effect. One based on constraint effects and another that made use of statistical weakest link concepts to explain the probability to find a cleavage initiator site at the crack front. The first fails to explain the observed scatter.

As the result of many years of investigations, which began in the 1980s decade, and based mainly on the works of Wallin, ASTM has standardized the determination of a temperature reference (T_0) for the fracture toughness characterization of ferritic steels in this region by means of a MC. This function gives the variation of K_{Jmean} with temperature, for 1T specimen size, and is based on a 3P-W probability distribution, with two of them fixed.

Despite the fact that this MC is a huge technological advantage, there are many aspects that need a deeper analysis, including

- the relationship between Weibull shape parameters when *J* or *K* results are used,
- size effect and validity of the specimen sizes conversion imposed in the ASTM standard,
- the validity of a model based only on statistical effect without taking into account the constraint.

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