# The Elusive Temperature Dependence of the Master Curve

# <u>Kim Wallin</u>

VTT Materials and Built Environment, P.O. Box 1000, FI-02044 VTT, Espoo, Finland Kim.Wallin@vtt.fi

Abstract The Master Curve methodology for describing cleavage fracture toughness, scatter, size-effects and temperature dependence has been standardized in ASTM E1921. The scatter and size-effects predicted by the method are based on theory, whereas the temperature dependence is the result of empirical observations. The reason for the seemingly nearly invariant temperature dependence of the cleavage fracture toughness of different steels has until now eluded theoretical explanations. The standard fracture toughness temperature dependence is expressed in terms of the normalization fracture toughness K<sub>0</sub>. However, K<sub>0</sub> is really the product of three separate parameters, K<sub>min</sub>, K<sub>0i</sub> and P(K<sub> $\infty$ </sub>), all of which are temperature dependent. K<sub>min</sub> is related to the steepness of the stress distribution in front of the crack, K<sub>0i</sub> is connected to the likelihood of initiation and P(K<sub> $\infty$ </sub>) describes the likelihood of cleavage crack propagation in a unified stress field. This presentation gives some more insight into the factors that lead to the experimentally observed temperature dependence. Finally, a new more material specific temperature dependence usable instead of the standard expression is given.

Keywords Master Curve, Cleavage fracture, Temperature dependence

### **1. Introduction**

The Master Curve (MC) method is a statistical, theoretical, micromechanism based, analysis method for fracture toughness in the ductile to brittle transition region. The method, originally developed at VTT simultaneously account for the scatter, size effects and temperature dependence of fracture toughness.

The method has been successfully applied to a very large number of different ferritic steels and it forms the basis of the ASTM testing standard for fracture toughness testing in the transition region (ASTM E1921-12).

#### **1.1.** The basic Master Curve

The MC approach is based on a statistical brittle fracture model, which gives for the scatter of fracture toughness in the form of Eq. (1) [1].

$$P[K_{IC} \le K_{I}] = 1 - \exp\left(-\left[\frac{K_{I} - K_{min}}{K_{0} - K_{min}}\right]^{4}\right),$$
(1)

In Eq. (1),  $P[K_{IC} \le K_I]$  is the cumulative failure probability,  $K_I$  is the stress intensity factor,  $K_{min}$  is the theoretical lower bound of fracture toughness and  $K_0$  is a temperature and specimen size dependent normalization fracture toughness, that corresponds to a 63.2% cumulative failure probability being approximately  $1.1 \cdot \overline{K}_{IC}$  (mean fracture toughness). The special form of Eq. 1 with  $(K_I - K_{min})^4$ , instead of  $K_I^4 - K_{min}^4$ , comes from a conditional crack propagation criterion, which makes the MC to deviate from a simple weakest link model of the weakest link. The model predicts a statistical size effect of the form of Eq. (2) [1].

$$K_{B_{2}} = K_{\min} + \left[K_{B_{1}} - K_{\min}\right] \cdot \left(\frac{B_{1}}{B_{2}}\right)^{1/4},$$
(2)

The parameters B<sub>1</sub> and B<sub>2</sub> correspond to respective specimen thickness (length of crack front).

On the lower shelf of fracture toughness ( $K_{IC} \ll 50 \text{ MPa}\sqrt{m}$ ) the equations may be inaccurate. The model is based upon the assumption that brittle fracture is primarily initiation controlled, even though it contains the conditional crack propagation criterion. On the lower shelf, the initiation criterion is no longer dominant, but the fracture is completely propagation controlled. In this case there is no statistical size effect (Eq. 2) and also the toughness distribution differs (not very much) from Eq. (1). In the transition region, where the use of small specimens becomes valuable, Eqs. (1) and (2) are valid.

For structural steels, a "Master Curve" describing the temperature dependence of fracture toughness is assumed in the form of Eq. (3).

$$\mathbf{K}_{0} = 31 + 77 \cdot \exp(0.019 \cdot [\mathbf{T} - \mathbf{T}_{0}]), \qquad (3)$$

 $T_0$  is the transition temperature (°C) where at which the mean fracture toughness, corresponding to a 25 mm thick specimen, is 100 MPa $\sqrt{m}$  and  $K_0$  is 108 MPa $\sqrt{m}$ .

The original data used to define Eq. (3) are shown in Fig. 1. It should be pointed out that the temperature dependence is purely empirical, even though it has been found to provide a rather good description of a large number of structural steel. The assumption is that the dislocation mobility in the ferrite matrix controls the temperature dependence. So far, attempts to provide a theoretical derivation of the temperature dependence have not been successful. One reason for this may be that most theoretical models only deal with cleavage fracture initiation. However, it is not only the probability of initiation that is affected by temperature. The theoretical temperature dependence is considered next.

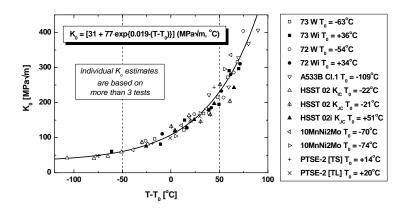


Figure 1. Original data used to define the temperature dependence of the MC. Each point denotes a  $K_0$  estimate based on more than three tests [1].

#### 1.2. Basis for the temperature dependence

The different possible mechanisms of cleavage fracture are qualitatively rather well known. Primarily the initiation is a critical stress controlled process, where stresses and strains acting on the material produce a local failure, which develops into a dynamically propagating cleavage crack. The local "initiators" may be precipitates, inclusions or grain boundaries, acting alone or in combination. An example of a typical cleavage fracture initiation process is presented schematically in Fig. 2. The first step involves the cracking of a precipitate or inclusion (sometimes, it may also be a grain boundary or grain triple point). The second step consists of the carbide size micro-crack propagating into the surrounding matrix and the third step consists of the grain-size crack propagating into neighboring grains. The two first steps are mainly affected by the particle size and the local stress and strain at the initiation site. The third step, however, is also affected by the stress gradients in the vicinity of the initiation site, since the third step covers a larger material volume.

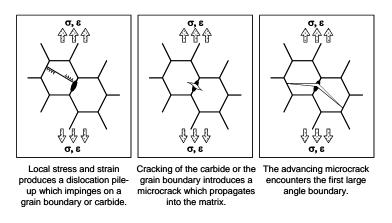


Figure 2. Schematic presentation of the necessary steps for cleavage fracture initiation [1].

Depending on loading geometry, temperature, loading rate and material, different steps are more likely to be most critical. For structural steels at lower shelf temperatures and ceramics, in the case of cracks where the stress distribution is very steep, steps II and III are more difficult than initiation and they tend to control the fracture toughness. At higher temperatures, where the steepness of the stress distribution is smaller, propagation becomes easier in relation to initiation and step I becomes more and more dominant for the fracture process. The temperature region where step I dominates is usually referred to as the transition region.

On the fracture surface of a specimen with a fatigue crack this is usually seen as a difference in the number of initiation sites visible on the fracture surface (Fig. 3). At lower shelf temperatures, numerous initiation sites are visible, whereas at higher temperatures, corresponding to the transition region, only one or two initiation sites are seen. In the case of notched or plain specimens, only a few initiation sites are seen even on the lower shelf. This is due to that, for cracks, the peak stresses are very high virtually from the beginning of loading, whereas for notched and plain specimens, the peak stresses increase gradually during loading. The fracture surface appearance is an effective tool in the decision if the material is on the lower shelf or in the transition region. The region has an implication on the macroscopic statistical behavior of cleavage fracture and is therefore also affecting the application of the fracture toughness test results.

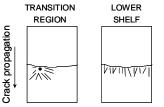


Figure 3. Typical cleavage fracture surfaces for fatigue pre-cracked specimens indicating differences in transition region and lower shelf behavior [1].

Due to the complexity of the cleavage process, a statistical model is needed to understand the effect of the different steps on the temperature dependence.

# 2. Statistical modeling of cleavage fracture initiation

The basis of a general statistical model is the following. It is assumed that the material in front of the crack contains a distribution of possible cleavage fracture initiation sites i.e. cleavage initiators. The cumulative probability distribution for a single initiator being critical can be expressed as Pr{I} and it is a complex function of the initiator size distribution, stress, strain, grain size, temperature, stress and strain rate etc. The shape and origin of the initiator distribution is not important in the case of a "sharp" crack. The only necessary assumption is that no global interaction between initiators exists. This means that interactions on a local scale are permitted. Thus a cluster of cleavage initiations may be required for macroscopic initiation. As long as the cluster is local in nature, it can be interpreted as being a single initiator. All the above factors can be implemented into the initiator distribution and they are not significant as long as no attempt is made to determine the shape and specific nature of the distribution. A quantitative description of the initiator distribution is also hindered by the statistical variation in stress and strain between grains and laths. Further, also the local orientations would need to be known. This is one reason why all present cleavage fracture models have had difficulties in connecting the models to real microstructural variables.

If a particle (or grain boundary) fails, but the broken particle is not capable of initiating cleavage fracture in the matrix, the particle sized microcrack will blunt and a void will form. Such a void is not considered able to initiate cleavage fracture. Thus, the cleavage fracture initiator distribution is affected by the void formation, leading to a conditional probability for cleavage initiation ( $Pr{I/O}$ ). The condition being that the cleavage initiator must not have become a void. The cleavage fracture process contains also another conditional event, i.e. that of propagation. An initiated cleavage crack must be able to propagate through the matrix in order to produce failure. Thus the conditional probability will be that of propagation after initiation ( $Pr{P/I}$ ). The cleavage fracture initiation process can be expressed in the form of a probability tree (Fig. 4).

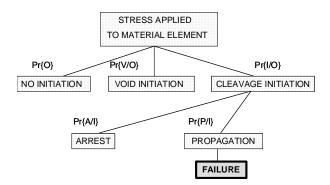


Figure 4. Probability tree for cleavage fracture [1].

#### 2.1. Probability of initiation

For a "sharp" crack in small scale yielding the stresses and strains are described by the HRR field. One property of the HRR field is that the stress and strain distribution is self-similar and another that the stresses and strains have an angular dependence. The term "small scale yielding" is in this derivation used to describe the loading situation where the self-similarity of the stress field remains unaffected by loading. For such a situation, it has been shown, by weakest link statistics, that the probability of initiation alone can be expressed in the form of Eq. (4) [1].

$$P_{f} = \Pr\{I/O\} = 1 - \exp\left\{-\frac{B}{B_{0}} \cdot \left(\frac{K_{I}}{K_{0i}}\right)^{4}\right\},$$
(4)

 $B_0$  is a freely definable normalization crack front length and  $K_{0i}$  corresponds to a cumulative initiation probability of 63.2%.

#### 2.2. Conditional cleavage propagation

Eq. (4) would imply that an infinitesimal  $K_I$  value might lead to a finite failure probability. This is not true in reality. For very small  $K_I$  values the stress gradient becomes so steep that even if cleavage fracture can initiate, it cannot propagate into the surrounding and other adjacent grains, thus only causing a zone of microcracks in front of the main crack. If propagation in relation to initiation is very difficult, a stable type of fracture may evolve. This is an effect often seen with ceramics. The need for propagation leads to a conditional crack propagation criterion, which causes a lower limiting  $K_{min}$  value below which cleavage fracture is impossible. For structural steels in the lower shelf temperature range, the fracture toughness is likely to be the controlled by the inability of propagation (Fig. 3).

The question regarding propagation alters the above pure weakest link type argument somewhat. It means that initiation is not the only requirement for cleavage fracture, but additionally a conditional propagation requirement must be fulfilled. Thus one must examine the probability of cleavage initiation during a very small load increment, assuming that no initiation has occurred before. Such a probability constitutes a conditional event and the resulting function is known as the hazard function. When the hazard function for initiation is multiplied by the conditional probability of propagation ( $Pr{P/I}$ ), the cumulative failure probability including propagation becomes thus as Eq. (5) [1].

$$P_{f} = 1 - \exp - \int_{K_{min}}^{K_{I}} \Pr\{P / I\} \cdot \frac{B}{B_{0}} \cdot \frac{4 \cdot K_{I}^{3}}{K_{0i}^{4}} \cdot dK_{I},$$
(5)

There are two requirements for  $Pr\{P/I\}$ . It must be an increasing function starting from  $K_{min}$  and for large  $K_I$  values it must saturate towards a constant probability corresponding to a uniform stress denoted by an infinite stress intensity factor  $K_{\infty}$ . One possible form of  $Pr\{P/I\}$  is given by Eq. (6). Other possible forms have also been discussed in e.g. [1].

$$\Pr\{P/I\} = P(K_{\infty}) \cdot \left(1 - \frac{K_{\min}}{K_{I}}\right)^{3},$$
(6)

All the possible equations are functions growing from 0 to  $P(K_{\infty})$ , where  $P(K_{\infty})$  is a number smaller than 1. The constant  $P(K_{\infty})$  reflects the finite probability of crack propagation even in a uniform stress field, being due to a possible miss-orientation between the micro-crack and the possible cleavage crack planes and the need to cross a grain boundary.  $P(K_{\infty})$  will increase with increasing stress and decrease with increasing temperature.

Insertion of Eq. (6) into Eq. (5) leads to the equation for the cumulative cleavage fracture probability including the conditional propagation criteria, (Eq. 7).

$$P_{f} = 1 - \exp\left\{-\frac{B}{B_{0}} \cdot \frac{P(K_{\infty})}{K_{0i}^{4}} \cdot \left(K_{I} - K_{\min}\right)^{4}\right\},\tag{7}$$

Eq. (7) is equivalent to the basic MC expression given by Eqs. (1) and (2). Eq. (7) shows that the basic MC  $K_0$  parameter is actually a complex parameter having the detailed form of Eq. (8).

$$K_{0} = \frac{K_{0i}}{P(K_{\infty})^{1/4}} + K_{\min} , \qquad (8)$$

 $K_0$  is really the product of three separate parameters, all of which are temperature dependent. The parameter  $K_{min}$  is usually only weakly temperature dependent, since it is mainly a result of the steepness of the crack stress distribution and the effective surface energy. The increase in  $K_{min}$  usually occurs at temperatures where  $K_0$  already is close to upper shelf. The temperature dependence of  $K_{0i}$ , is a function of the changes in initiator distribution with temperature and the materials yield stress. The temperature dependence connected to  $K_{0i}$  should mostly be controlling at low temperatures, where the yield stress sensitivity to temperature is large. This leaves the probability of cleavage crack propagation in a unified stress field,  $P(K_{\infty})$ , as the likely parameter describing most of the temperature dependence in the transition region. This is also in line with the fact that the crack arrest toughness has very similar temperature dependence as  $K_0$  [1].

### **3. Discussion**

Considering the complicity of  $K_0$ , one should not assume that all ferritic steels have exactly the same temperature dependence. This is especially the case for such steels, where the chemistry affects the dislocation mobility in the ferrite matrix. E.g. high nickel steels, even though ferritic, are likely to show different temperature dependencies, since nickel is known to affect the materials crack arrest properties favorably. To study the possible variation in the fracture toughness temperature dependence between different structural steels, 82 data sets each with at least 20 significant samples have been fitted with the MC, with  $K_0$  in the form of Eq. (3), where the parameter C (normally  $0.0019^{\circ}C^{-1}$ ) is a variable. The median fracture toughness curves are shown in Fig. 5. The figure shows also the theoretical statistical uncertainty related to a sample size of 20, if the parameter corresponds to  $C = 0.019^{\circ}C^{-1}$ . Even though nearly 80% of the estimates fall within this region, there are materials that clearly deviate from the standard MC.

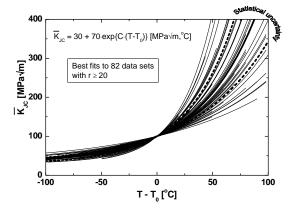


Figure 5. Compilation of median fracture toughness temperature dependence estimates for a large variety of structural steels having more than 20 significant samples. The thick full line indicates the standard MC and the dashed lines indicates the statistical 5% and95% uncertainty limits related to a sample size of 20. [1].

A three-dimensional fit of the temperature dependence can be expressed in the form of Eq. (9) [1], even though other similar forms provide practically the same accuracy. Regardless of the exact choice of function, the trend is clear. Yield stress has a rather insignificant effect on the temperature dependence whereas the transition temperature has a more significant effect.

$$C\left[^{\circ}C^{-1}\right] \approx 0.008 + \left(\frac{20.9 \text{ MPa}}{\sigma_{Y}}\right)^{2.24} + \left(\frac{0.6^{\circ}C}{T_{0} + 273^{\circ}C}\right)^{0.77},$$
(9)

The reasons for the effect of  $T_0$  on the shape of the transition curve, may partly be due to fact that the difference between initiation toughness and crack arrest toughness are affected by  $T_0$  (See [1]) or it can be partly related to a rough connection between upper shelf toughness and  $T_0$ . The difference in initiation toughness and crack arrest toughness would affect  $K_0$  by affecting  $K_{min}$  and  $P(K_{\infty})$ , in relation to  $K_{0i}$ , whereas the upper shelf toughness would control the amount of ductile tearing prior to cleavage fracture and would thus affect  $K_{0i}$ .

Overall, the analysis indicates that the use of the standard MC with a fixed  $C = 0.019^{\circ}C$ -1 is well applicable for steels with  $T_0$  in the range  $-100^{\circ}C$ ... $+50^{\circ}C$ . Since the MC is fitted to the data in the temperature range  $T_0$ -50°C to  $T_0$ +50°C, it will provide a satisfactory description of the fracture toughness in this temperature region. Any deviations in transition curve steepness will be adjusted for by shifts in  $T_0$  and the overall description of the data in that region is adequate. However, if the materials  $T_0$  value or the application temperature. Due to the considerable statistical uncertainty connected to parameter C, it is not recommended to experimentally estimate it for a single application. As long as there are test results not too far from the application temperature, the standard MC can well be used. As a sensitivity analysis, the standard MC analysis can be complemented with an analysis using Eq. (9). In this case, a first estimate of  $T_0$  is obtained with a standard analysis, which is then repeated using the C value obtained from Eq. (9). This way, it is not necessary to increase the number of tests from a standard analysis. An experimental estimation of C requires 20 to 40 specimens. A bigger source of uncertainty in the MC analysis, than the transition curve shape, is the possible material in-homogeneity.

Most cleavage fracture local approach models have adopted the basic MC temperature dependence as a calibrator for the models, since they only consider  $K_{0i}$  and do not thus account for the effect of the conditional propagation criterion. Only one model claims to be able to theoretically correctly describe the material-to-material variation of the temperature dependence. This model is known as the Unified Curve method based on the Prometey probabilistic model for cleavage fracture [2]. The model, like most others, only predicts  $K_{0i}$ , even though the Unified Curve has adopted the MC form with a constant  $K_{min}$  parameter. The Prometey model does not, however, predict a  $K_{min}$ . The temperature dependence of the Prometey model comes mainly from two parameters: <sup>1)</sup>the thermal part of the yield strength's temperature dependence and <sup>2)</sup>the characteristic strength of initiating carbides ( $\mathscr{O}_{Q}$ ). The effect of  $\mathscr{O}_{Q}$  is shown in Fig. 6 [2] where the other parameters have been calibrated to a Russian pressure vessel steel (2Cr-Ni-Mo-V), and kept constant. The difference between the figures a) and b) is the athermal part of the materials yield strength which in a) is 510 MPa and in b) 710 MPa and the Weibull modululs  $\eta$  which is 6 in a) and 12 in b). Even these very simple changes in the parameter are seen to produce a large difference in the predicted fracture toughness.

Any changes in the thermal part of the materials yield strength should, according to the model, have even a larger effect on the sensitivity of the model to used parameters. On top of this, the strongest sensitivity to temperature is, as seen in Fig. 6, above  $0^{\circ}$ C, where the thermal part of the yield strength becomes very small. The model is thus strongly dependent on the correct estimate of the thermal yield strength component in this temperature region. Considering this, it is surprising that this single material calibration has been applied to develop the so called Unified Curve method and claimed to be correct for all kinds of steels. Scientifically, the claim is clearly invalid. The model is incomplete, and since it does not account for the conditional propagation criterion it cannot be used to predict the temperature dependence of fracture toughness. The temperature dependence has been calibrated only for one material and therefore, similar to other local approach models considering only  $K_{0i}$ , the model cannot be used to predict a quantitative fracture toughness temperature dependence.

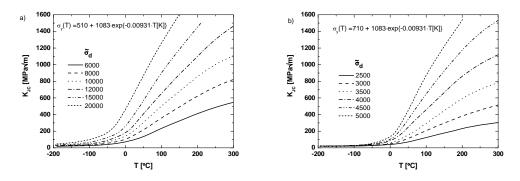


Figure 6. Two examples of the predictions based on the Prometey model [2]. The difference in the figures is the athermal part of the materials yield strength and the Weibull modululs ( $\eta = 6$  vs. 12). Changing the thermal part of the materials yield strength would greatly enhance the differences.

### 4. Summary and Conclusions

The Master Curve methodology for describing cleavage fracture toughness, scatter, size-effects and temperature dependence has been standardised in ASTM E1921. The scatter and size-effects predicted by the method are based on theory, whereas the temperature dependence is the result of empirical observations. The reason for the seemingly nearly invariant temperature dependence of the cleavage fracture toughness of different steels has until now eluded theoretical explanations. The standard fracture toughness temperature dependence is expressed in terms of the normalization fracture toughness  $K_0$ . However,  $K_0$  is really the product of three separate parameters,  $K_{min}$ ,  $K_{0i}$  and  $P(K_{\infty})$ , all of which are temperature dependent.

 $K_{min}$  is related to the steepness of the stress distribution in front of the crack,  $K_{0i}$  is connected to the likelihood of initiation and  $P(K_{\infty})$  describes the likelihood of cleavage crack propagation in a unified stress field.

 $K_{min}$ , despite its temperature dependence, does not explain the temperature dependence of  $K_0$ , since the increase in  $K_{min}$  usually occurs at temperatures where  $K_0$  already is close to upper shelf.

The same is the case for the initiation toughness  $K_{0i}$ , which mainly should be a function of the initiator distribution and the materials yield stress. The temperature dependence connected to  $K_{0i}$  should mostly be effective at low temperatures, where the yield stress sensitivity to temperature is large.

This leaves the probability of cleavage crack propagation in a unified stress field,  $P(K_{\infty})$ , as the likely parameter describing most of the temperature dependence. This is also in line with the fact

that, the crack arrest toughness has very similar temperature dependence as K<sub>0</sub>.

This presentation gave some more insight into the factors that lead to the experimentally observed temperature dependence. Finally, a new more material specific temperature dependence usable instead of the standard expression has been given.

Finally it has been shown that the so called Unified Curve method, based on the Prometey cleavage fracture model is scientifically invalid and should not be used to predict a quantitative fracture toughness temperature dependence.

#### Acknowledgements

This work has been part of the FAR project belonging to the SAFIR 2014 research program funded by VTT and by the State Nuclear Waste Management Fund (VYR), as well as other key organizations. The present work is connected to the quantification of constraint effects in brittle and quasi-brittle materials.

#### References

- [1] K.R.W. Wallin, Fracture toughness of engineering materials estimation and application, EMAS Publishing, Warrington UK, 2011.
- [2] B.Z. Margolin, A.G. Gulenko, V.A. Nikolaev, L.N. Ryadkov, A new engineering method for prediction of the fracture toughness temperature dependence for RPV steels, International Journal of Pressure Vessels and Piping, 80, (2003), 817–829.